UCRL-52532, Vol. 4, Pt. 4

Computer automation of continuous-flow analyzers for trace constituents in water

Volume 4. Description of program segments

Part 4. TAACAL

R. W. Crawford

November 2, 1979

Lawrence Livermore Laboratory

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FOREWORD

There are 13 programs used in the computer automation of continuous-flow analyzers for trace constituents in water. Each program is published separately as a part of this volume:

Part 1. TAAIN
Part 2. TAAINRE
Part 3. TAASTART
Part 4. TAACAL
Part 5. TAA
Part 6. TAAQCOP
Part 7. TAA01
Part 8. TAA02
Part 9. TAA03
Part 10. TAA04
Part 11. TAARESTART
Part 12. Utility Programs (TAAPRINT, TAAPEAK, TAAFILE)
Part 13. Assembly Language Code

CONTENTS

Computer automation of continuous-flow analyzers for trace constituents in water

ABSTRACT

This report describes TAACAL, one of a series of computer programs necessary in automating the Technicon AutoAnalyzer. TAACAL measures the calibration standards and sets up the calibration curve. A flow chart and sequence list that describes and illustrates each logical group of coding, and a description of the contents and functions of each section and subroutine in the program is included. In addition, all arrays, strings, and variables are listed and defined, and a program listing with a complete list of symbols and references is provided.

PROGRAM DESCRIPTION

TAACAL is the first of the computer programs used by the operator of the Technicon AutoAnalyzer that takes readings of the Analyzer output. The operator has used previously called programs interactively to store the operating parameters and descriptive information. TAACAL performs the next step—calibration of the instrument. The calibration standards are measured, and the coefficients of the calibration polynomial are calculated; these relate the instrument signal to the sample concentration.

The pattern of samples to be presented to the analyzer was set up with the TAAIN program, which is Part 1 of this series of descriptions of the program segments.[1] This sample wheel pattern is reproduced here as Fig. 1. The first sample wheel in a run is loaded with the set standards and is followed by the calibration standards; this is called the calibrate pattern. Following this are groups of quality control (QC) patterns containing blanks, check standards, samples, spiked samples, and duplicates, as previously defined by the operator interacting with TAAIN. TAACAL is primarily concerned with the calibrate pattern.

The programs presented in this series of documents all operate with up to three channels of Technicon AutoAnalyzers. The program for the AutoAnalyzer-II is described here in detail. Changes necessary for operating with the older AutoAnalyzer-I are explained in a separate section of this report. To operate with up to six channels, the changes needed are minor, and they are mostly concerned with the formatting of input and output. Any changes required in the operation of another brand of continuous-flow analyzer may be more difficult to implement.

For multi-channel operation, the sample is aspirated from the sample container and split into several streams, each of which is subjected to different chemistries according to the sample species. The length of each branch of the reaction train is optimized for the particular analysis. Since these lengths are different for each analyte, the signals from the colorimeters are out of phase. It is likely that the signal from one colorimeter for a sample may precede or follow quite a different sample from another colorimeter. Data are carefully organized on the computer disk to prevent scrambling of sample analyses. The file structure used is described in Volume 2 of this series of reports.

Before the TAACAL program is initiated, the real-time assembly-language program is placed in Search mode by TAASTART. TAASTART chains to TAACAL, which initializes variables and issues a CALL 18;[2] this call passes peak-height data to the BASIC program. Since no data are yet available, the real-time code puts TAACAL into a waiting state and permits it to be removed from core. As

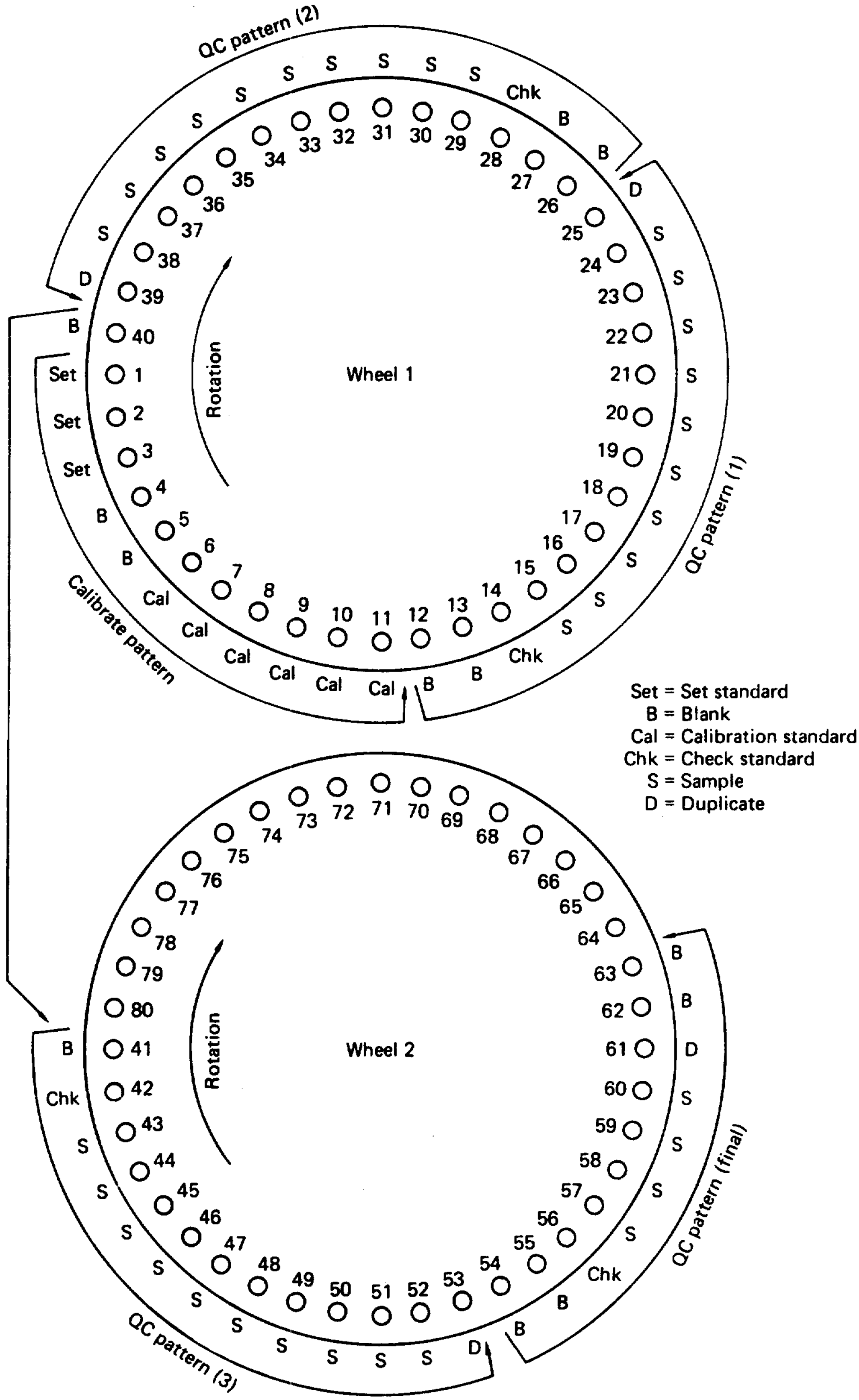

FIG. 1. Pattern for a sample wheel as prepared for the AutoAnalyzer II.

soon as a peak has been recorded by the real-time code from any of the colorimeters, TAACAL is restarted at the statement following CALL 18. Two arrays are returned to TAACAL, E(x), containing the channel and peak numbers, and D(x), containing the 35 data-points that characterize the top of the peak. The TAAID.xx file that is appropriate to this channel is opened, and the record describing the sample that corresponds to this peak number is retrieved.* The first item in this record is T, or type of solution. According to the value of T, the program then branches to the appropriate one of the five major routines.

MAJOR SUBROUTINES

Each of these major routines finds the peak top, smooths the data, corrects for the baseline, and stores the peak-height value in the record. These routines also check to see if all channels of the current sample have been recorded and, if so, display the data on the terminal.

Set-Standard Samples

If T is 1, the sample is a Set standard. These are used by the program to establish the initial time and the sample-interval timing, and they are used by the operator to adjust the calibration of the colorimeters. For the Technicon printer, which is not a part of the computerization, the initial time must also be established by pressing the START button on the printer. It is critical that this initial time be accurately established. The time interval between the "knees" on the peaks from the second and third Set standards is compared with the operator-entered expected interval, and an error expressed in seconds is displayed. Errors of less than eight seconds are not significant. Errors greater than eight seconds may indicate either an error in entering the number of samples per hour, a timing problem in the sampler, or misshapen peaks.

Blank Samples

If T is 2, the sample is a Blank. This type establishes the initial baseline for the Calibration standards. The lower of the two Blanks following the Set standards is used as a constant baseline to calculate the initial peak-height values for the Calibration standards. The lower of the two Blanks after the Calibration standards is used with the previous value to establish the slope of the baseline. The values for the Calibration standards are then recalculated with the assumption of a linear baseline between the two pairs of Blanks. This linear baseline is also extrapolated forward to be used with the first quality-control pattern, as illustrated in Fig. 2.

The coefficients of the calibration polynomial are calculated using these corrected values for the peak heights. Because of the baseline slope, the values for the Calibration standards in Analog to Digital (A/D) converter units printed on the final report may be different from those printed during the run. The final report values are those used to calculate the coefficients of the calibration polynomial.

Calibration-Standard Samples

If T is 3, the sample is a Calibration standard. After all values are collected and corrected for the baseline, they are used to calculate the coefficients of the calibration polynomial

X = A + B*Y + C*Y↑2 + D*Y↑3 ,

where X is the concentration and Y is the measured peak-height value. The selection of a linear, quadratic, or cubic fit was made earlier in TAAIN. The standards are sorted into ascending concentration, so that they can be used in linear interpolation between calibration points.

A zero peak-height, zero-concentration datum is appended to the Calibration standards. If the operator has indicated a zero concentration for any of the standards, those standards are ignored. Since the zero-intercept A is rarely zero, all samples between zero and the least-concentrated standard are calculated by interpolation. This avoids the problem of explaining reported negative concentrations.

The lowest-order polynomial possible should be used. Many analyses give linear calibration

*The term *enter* means to type a value in on the terminal. It does not indicate what happens to the data. *Get* applies to memory and *retrieve* applies to disk files. The term *write* is used with memory. *Write file* and *store* are used with disk files. *Save* is reserved for storing a program on disk.

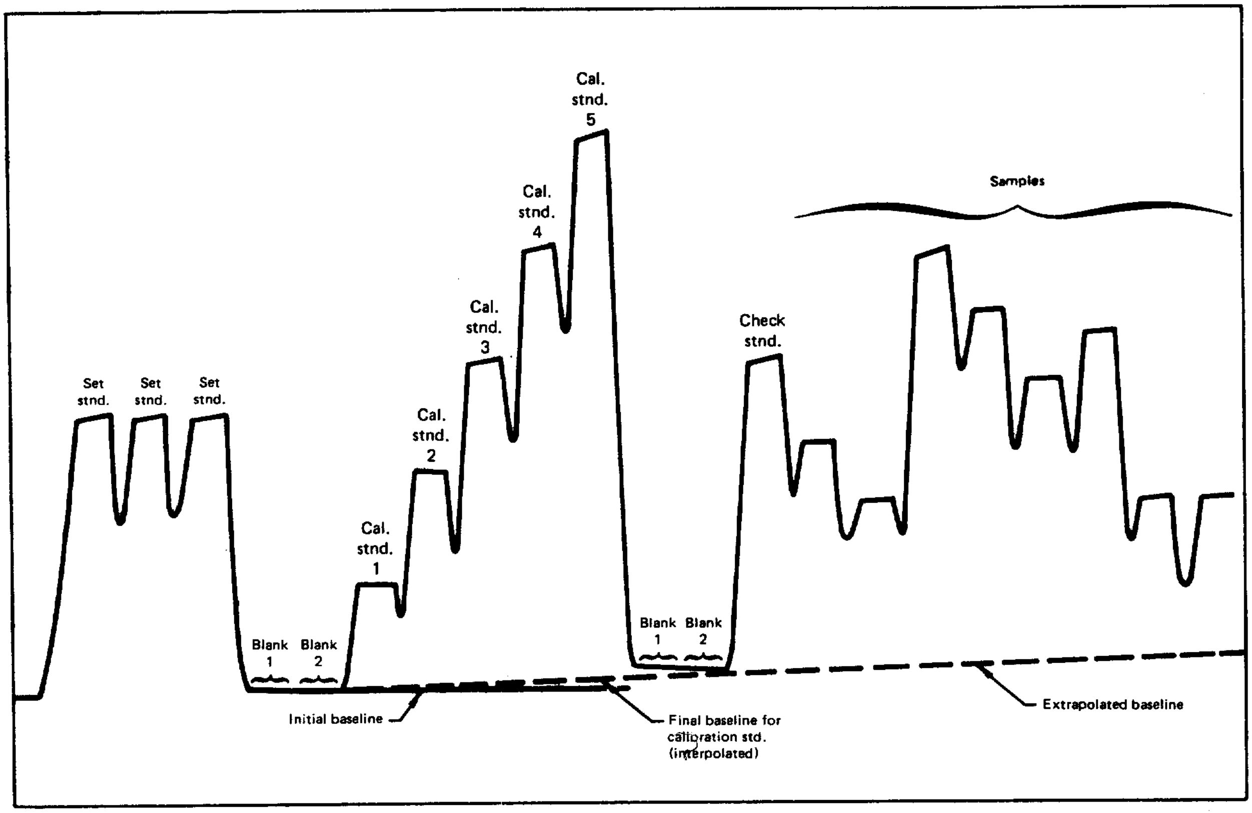

FIG. 2. Calibration scheme showing the use of Blanks to establish the baseline.

curves in the range of interest. Some other analytical methods exhibit some curvature at high concentrations and can be fitted with a quadratic. A few methods exhibit curvature at both low and high concentrations. These can be fitted with a cubic, although it is usually preferable to add a known amount of the analyte to one of the reagents to bring the least concentration of the sample into the linear range.

Two indications of the degree of goodness of fit are provided. The coefficient of determination is calculated at the same time as are the coefficients. For a perfect fit the coefficient is 1.00000. Most managers of analytical laboratories insist upon a value in excess of 0.999. Others accept values as low as 0.99. Occasionally a value greater than 1.0 is displayed because of round-off errors in the computer arithmetic, and it is accepted. The other indication of the goodness of fit is the print-out of both the stated concentration and the concentration of the standard as calculated from the polynomial. If these disagree by much, it is an indication of a bad or misidentified standard solution.

It is important to use sufficient numbers of different standards. Mathematically speaking, only one is needed for a linear fit, two for quadratic, and three for cubic, as 0,0 is always appended to the observed data. More than the minimum number must be used in order to detect problems, as the minimum number will always give a perfect fit. Choose the order of the polynomial on the basis of the known chemistry, since a higher-order polynomial can hide a problem.

TAACAL also calculates the coefficients of a quadratic that relates the slope of the peak-top to the peak-height. Ideally, all peaks should be a constant value across the top. This is often not the case with large peaks and is almost never the case with AutoAnalyzer-I equipment. These coefficients are used later to analyze peaks for noise, spikes, and skewness. The slope of lower-concentration peaks tends to be zero, while higher-concentration samples have much steeper peaks. A quadratic was found to fit the data adequately. This is discussed more fully in Part 5 of this series, which describes program TAA.

Check-Standard Samples and Unknowns

If T is 5, the sample is a Check standard, and if T is 6, the sample is an unknown. TAACAL finds, smooths, and stores the peak height for both of these cases. This was done because one or more of these may arrive through a shorter reaction train before the last blank on the longest reaction train has arrived. It does not display results or do quality control, functions which are done by TAA.

After the calibration pattern on all channels is completed, and the coefficients of all polynomials have been calculated and stored, TAACAL chains to TAA.

UNUSUAL ALGORITHMS USED

Peak-Finding

Because noise may occur at or near the tops of peaks, the program uses either 11 or 21 data points to determine the peak height. Because the tops of the peaks have a slope, it is important to locate these data points in a manner that is reproducible. The sharpest change in slope is at the end of the peak top, where sampling stopped and washing began. This change is the easiest to detect, and it is referred to as the "knee" of the peak.

The knee is found by starting at the last of the 35 data points and working back until the slope changes from negative to zero. Four data are tested each time, so that if N is the number of the data point, and D[N]* is the value, we test to see if

$$D[N] > D[N-1] - 15, \text{ and}$$
$$D[N] > D[N-2] - 25, \text{ and}$$
$$D[N] > D[N-3] - 30 .$$

If all of these statements are true, then N is the location of the knee. By examining the typical data illustrated in Fig. 3, we see that for N = 35, the conditions are false. By decrementing N by one each time, we arrive at N = 26, for which the conditions are true.

*In this report, the BASIC notation is used, where brackets indicate an argument to a function or a list, a star (*) indicates the multiplication function, and a up-arrow (↑) stands for the exponential function.

There are several situations for which the peak-finding algorithm might fail, and we protect against them. If the peak is too small, the difference between adjacent data points on the trailing edge will be too small for the test. The problem is avoided by the assumption that any peak smaller than 10% of full scale is placed at the predicted location. A more complex problem occurs if there is a very small or nonexistent trailing edge. In this case, the knee appears to be at the very last point, the 35th. The program checks to see if the 35th point is at least 5% higher than the 20th point. This condition is illustrated in Fig. 4. If it is, the program checks for a reverse inflection using the same algorithm with positive signs rather than negative.

The peak-finding algorithm in TAA incorporates an additional step. In that program, the knee is located by searching in both directions. Calibration standards usually give good peaks so this refinement is not incorporated into TAACAL. The algorithm does not protect itself when the sampling rate is too fast. If this is the case, there will not be a steep enough slope to the trailing edge. This situation may be verified by running utility program TAAPEAK on the raw data. To correct the sampling rate, TAAIN must be restarted, with a smaller number being entered for the data rate.

Adjustment of Peak Timing

Over the course of a long run, the peak location may slip with respect to the 35-point data window. The standard peak location of 26 was chosen, so that when 21 points are used to define the peak-height, they can move to a place earlier in the window by 5 points before they fall out of the window. They may also move to a place later by 5 points, without losing ability to locate the knee.

If the knee is within 1 or 2 points of 26, no action is taken. If it is further away, a timing correction may be made by using CALL 19 between the first and second succeeding peaks. The BASIC program and the real-time code are running loosely coupled, so the correction cannot be made prior to the second following peak. For example, if the knee of peak No. 12 is at position 29, then the time between peaks 13 and 14 is reduced by the amount needed to move the expected knee of peak 14 to position 26. Peak 13 is not corrected, so its knee also appears at 29, and calls for a correction.

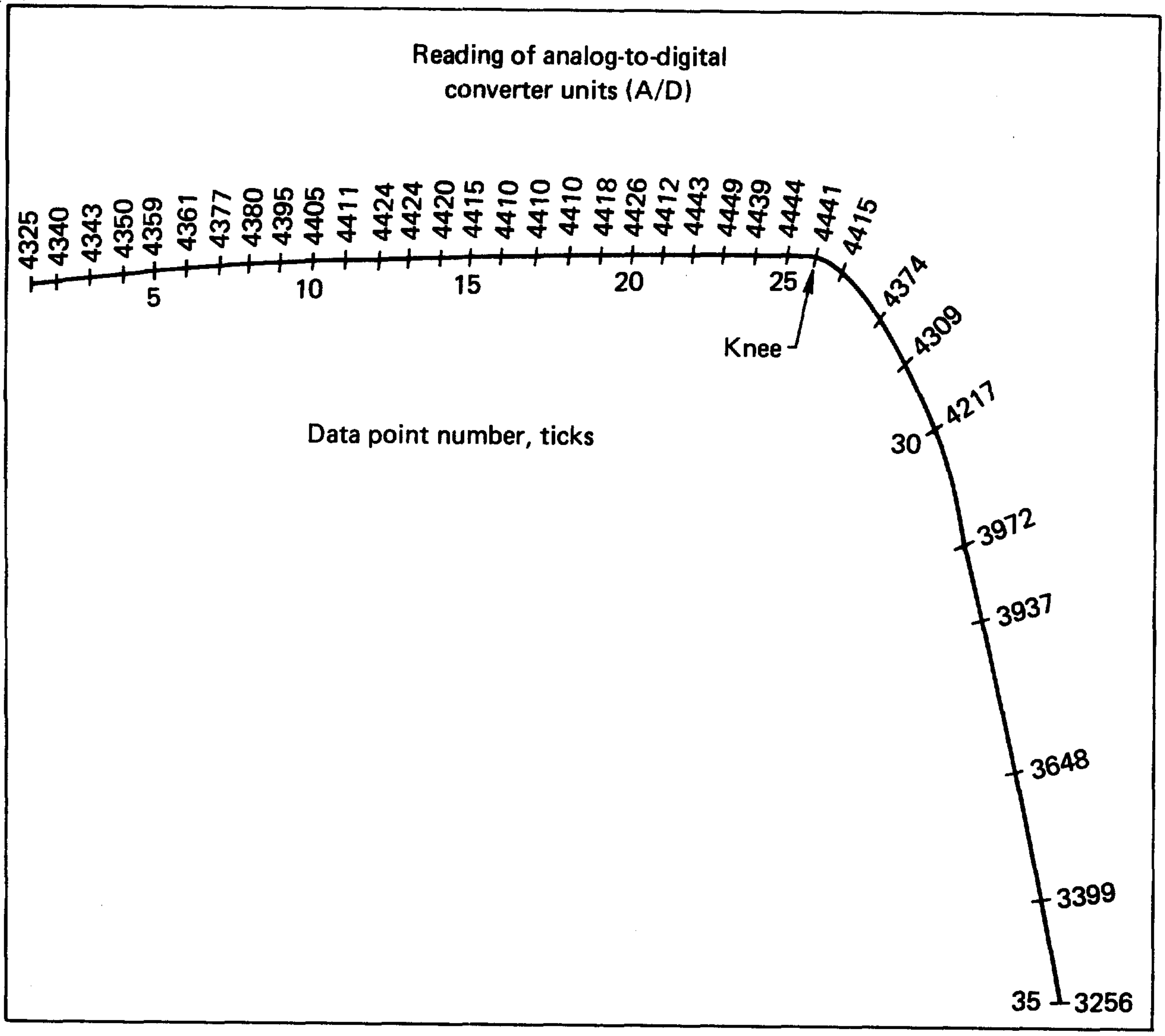

FIG. 3. **Typical 35 digitized data as shown for a peak; a "knee" occurs at n = 26.**

To avoid making the same correction twice, the program stores the peak number of the last peak calling for a correction in B[N,6], and logic is provided to suppress the redundant correction. If the calculated correction is between 3 and 5 locations, the full correction is made. To prevent oscillation, the maximum correction applied is 5, and the remaining correction will be made later by the algorithm.

CALL 19 uses a two-element array, M[1] is the A/D converter channel number, and M[2] is the number of 2/15-second ticks to be applied. CALL 19 has a one-time effect to move the window. The standard spacing between peaks is resumed after the correction is executed.

Slope of the Peak-Top

In order to properly correct for noise on the peak, it is important to know the slope of the top of the peak, a value determined for each Calibration standard. The form assumed is

$$Y = M*X + B\,.$$

As shown in Figs. 5a and 5b, this equation is fit by a change of variables, so that X = 0 is the center of the 11 or 21 points. In that case, M is given simply by

$$M = \frac{\Sigma(xy)}{\Sigma(x^2)}\,.$$

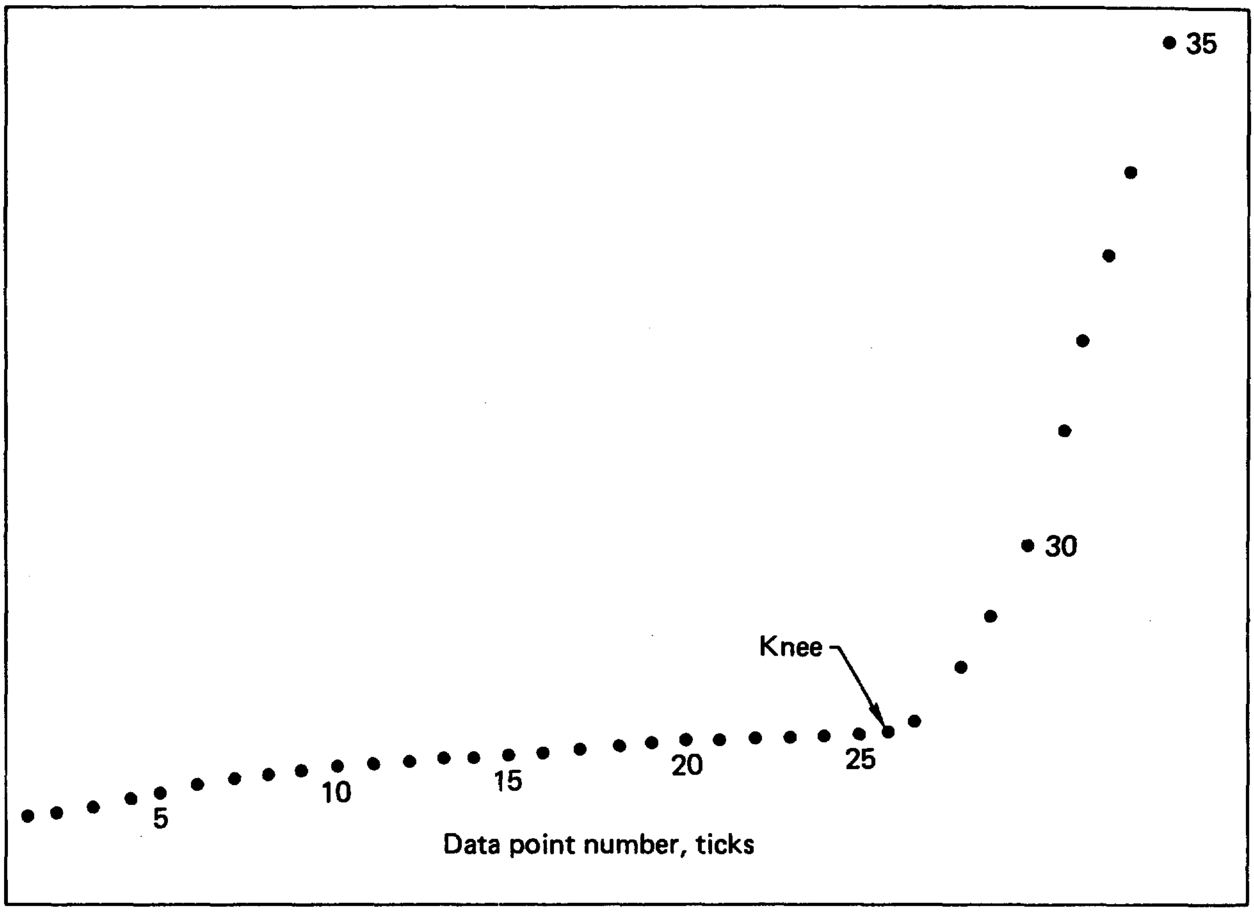

FIG. 4. A data array with a reverse inflection condition. The peak-finding algorithm can distinguish between peaks and reverse-inflection high-points.

This transformation also minimizes round-off error in the calculations. If D is the number of points used to define the peak height,

$$\Sigma(x^2) = \frac{(D-1)D(D+1)}{12} ,$$

which yields 110 for the denominator of M when 11 points are used, and 770 when 21 are used.

Peak-Smoothing

The tops of AutoAnalyzer peaks occasionally exhibit spikes or dips. In manual-mode operation, the operator corrects for these either by drawing a best line across the top of the peak and ignoring the noise, or by doing the equivalent mental operation. The peak-smoothing algorithm does the same operation for automated data. The average peak height F1 is calculated, with missing points excluded. The array R is filled with the expected height of each point, using the measured average and the expected slope of the peak-top.

In the first time through the standards, the expected peak-slope is the measured slope. On subsequent passes, and as noise spikes are eliminated, the estimate of the true peak-slope improves. The standard deviation of the points across the top of the peak is then calculated from the point-by-point difference between the actual data and that in the R array, as follows:

$$E3 = \sqrt{\frac{\Sigma(D_{meas} - R_{calc})^2}{J-2}}$$

Since we have two constants to determine, slope and average, the appropriate divisor for the standard deviation is $J - 2$, where J is the number of nonzero points.

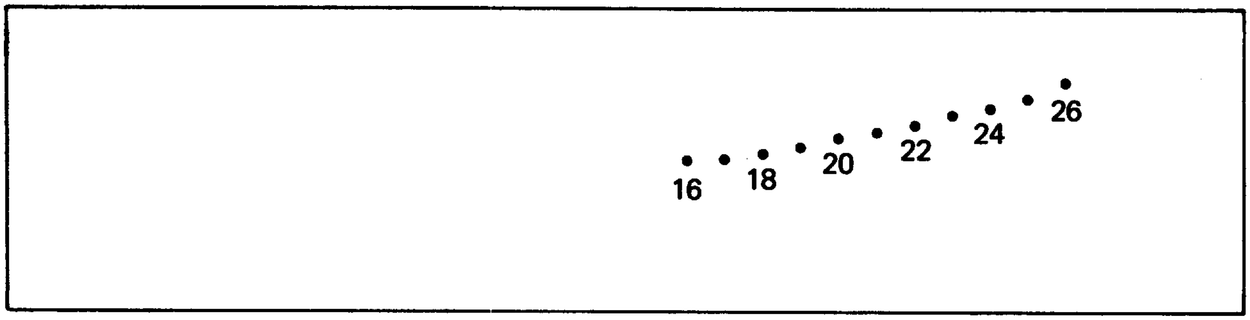

FIG. 5a. Peak data as it occurs in the array before the smoothing of the peak top.

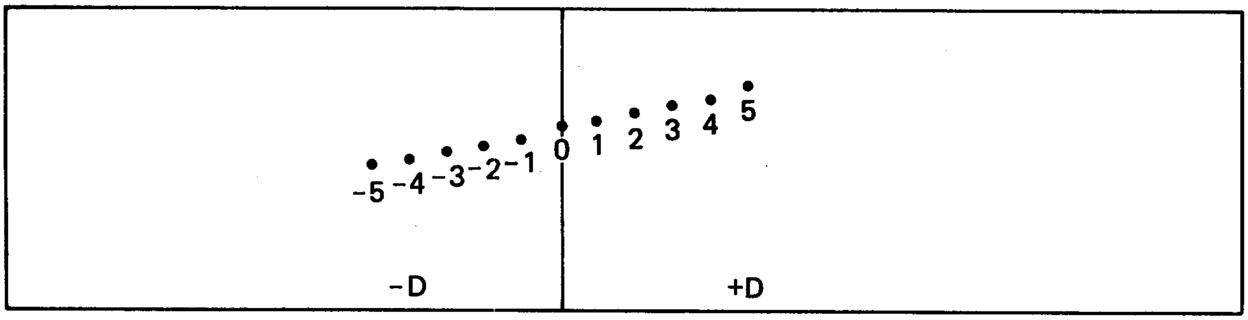

FIG. 5b. Peak data that has been centered on the X-axis for better determination of the slope of the peak top.

If the calculated standard deviation is less than the operator-defined acceptable deviation, no smoothing takes place, and the peak height is taken as the last value of the calculated R array. If the calculated standard deviation is too big, then the data is searched for differences which exceed 1.5 times the calculated deviation. In a normal distribution, about 2 out of 11 or 3 out of 21 data fail this test. Even if they are true data, excluding these few will not significantly bias the answer.

Each point that fails is replaced with the calculated value and counted. If no points are replaced, and if the standard deviation is less than 5 times that allowable, the sample is assumed to be fuzzy but unbiased, and it is accepted. If fewer than one-third of the data have been rejected, the operations of calculating the slope, average value, standard deviation, and casting out data are repeated. After a few iterations, either the peak will pass, or more than one-third of the points will have been rejected. In the latter case, the peak is labeled as noisy.

Fitting Polynomials to Data

The coefficients of the calibration polynomial are chosen by the least-squares method described in any basic statistics textbook. The program described here uses matrix methods that may be less familiar. Here, we review first the conventional method. If we select our polynomial as

$$y_j = a_1 + a_2 x_j + a_3 x_j^2 + \ldots + a_p x_j^{p-1}$$

where j is the pointer to one of the k data, and p−1 is the order of the polynomial, then the rules for the least-squares method tell us that the best fit to the data is a polynomial with coefficients obtained by solving the folowing set of equations:

$$\Sigma y = a_1 k + a_2 \Sigma x + \ldots + a_p \Sigma x^{(p-1)}$$

$$\Sigma xy = a_1 \Sigma x + a_2 \Sigma x^2 + \ldots + a_p \Sigma x^p$$

$$\Sigma x^{p-1} y = a_1 \Sigma x^p + a_2 \Sigma x^{p+1} + \ldots + a_p \Sigma x^{(2p-1)}$$

When matrix operations are available, we can solve these equations as shown below.

We set up a U matrix and H and A vectors with the following coefficients:

$$U = \begin{bmatrix} k & \Sigma x & \Sigma x^2 & \dots & \Sigma x^{p-1} \\ \Sigma x & \Sigma x^2 & \Sigma x^3 & \dots & \vdots \\ \Sigma x^2 & \Sigma x^3 & \Sigma x^4 & \dots & \vdots \\ \vdots & & & & \vdots \\ \Sigma x^{p-1} & \dots & \dots & \dots & \Sigma x^{2p-1} \end{bmatrix}$$

$$H = \begin{bmatrix} \Sigma y \\ \Sigma xy \\ \Sigma x^2 y \\ \vdots \\ \Sigma x^{p-1} y \end{bmatrix}$$

$$A = \begin{bmatrix} 1 \\ 2 \\ \vdots \\ p \end{bmatrix}$$

The least-squares equations are then

$$H = UA$$

and the solution for the coefficients is

$$A = U^{-1}H.$$

The coefficient of determination is defined as:

$$E7 = \frac{\Sigma(y_{calc} - y_{avg})^2}{\Sigma(y_{meas} - y_{avg})^2},$$

a standard measure of the goodness of fit. We may also write

$$E7 = \frac{\Sigma(y_{calc}{}^2 - ky_{avg}{}^2)}{\Sigma(y_{meas}{}^2 - ky_{avg}{}^2)},$$

as it is calculated in the program.

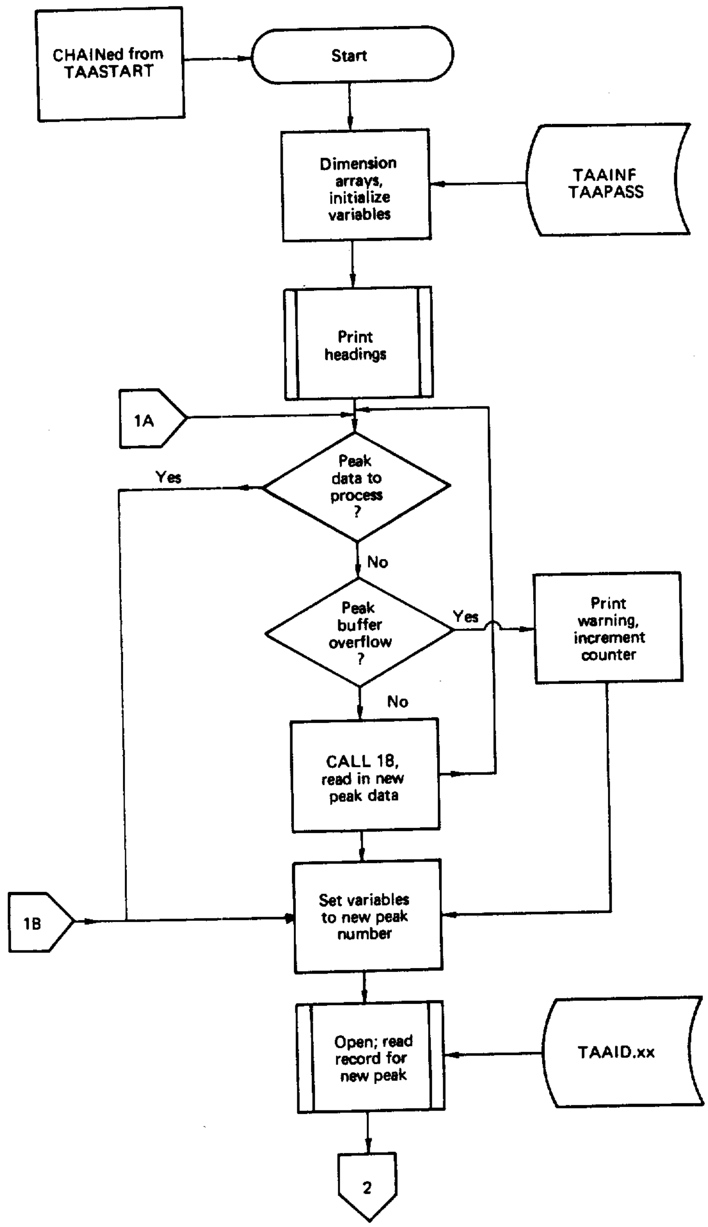

FIG. 6. Logic flow diagram of the TAACAL main program.

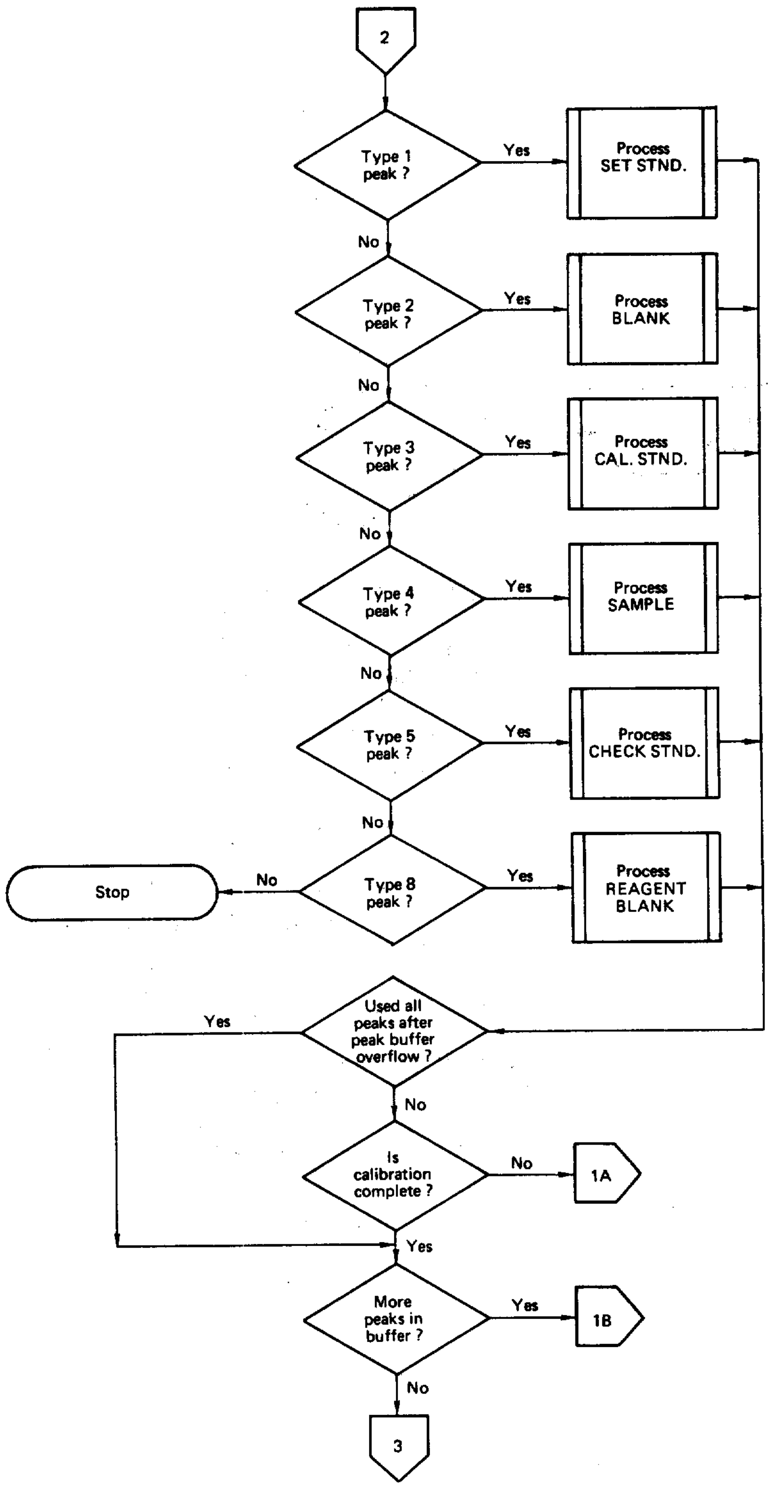

FIG. 6. (Continued.)

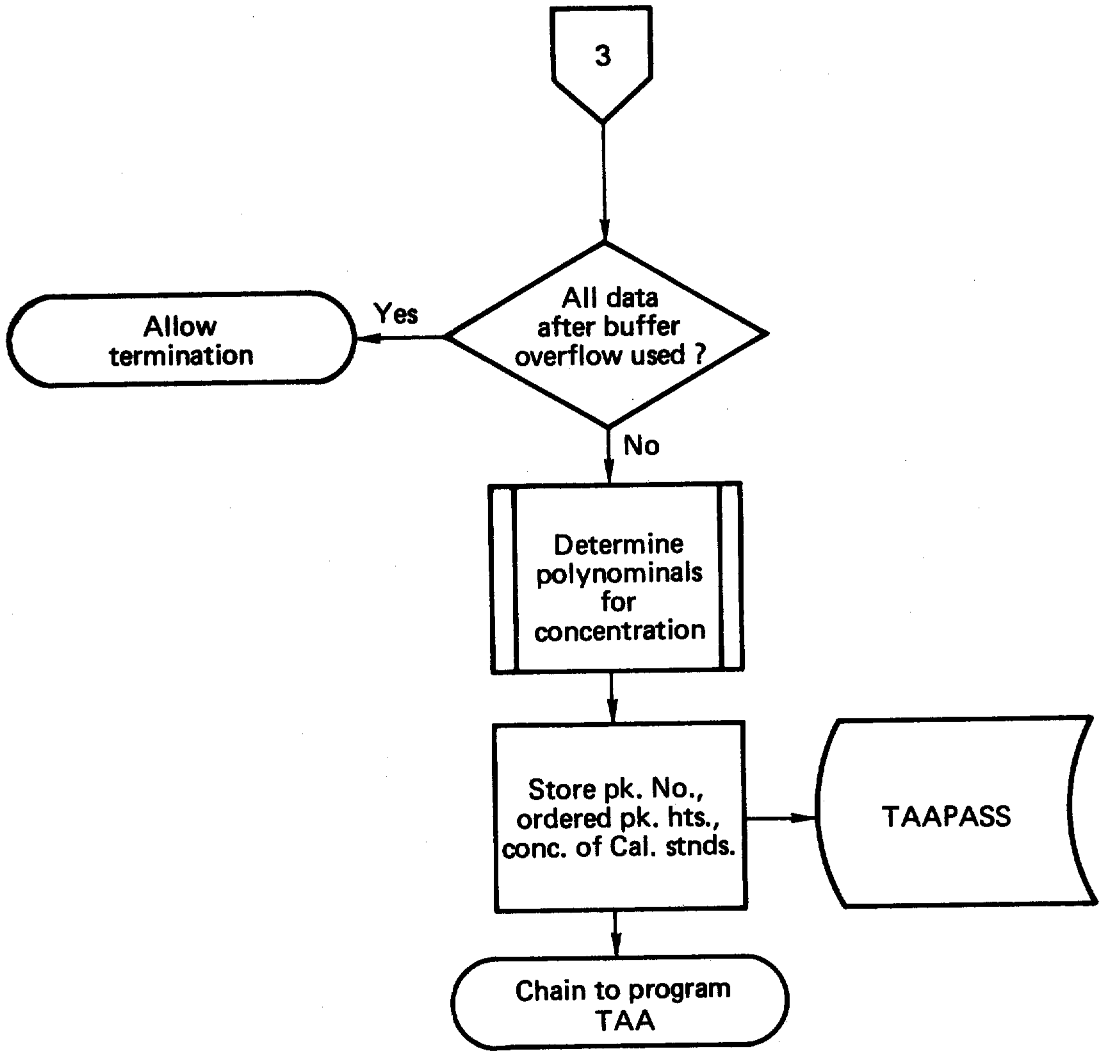

FIG. 6. (Continued.)

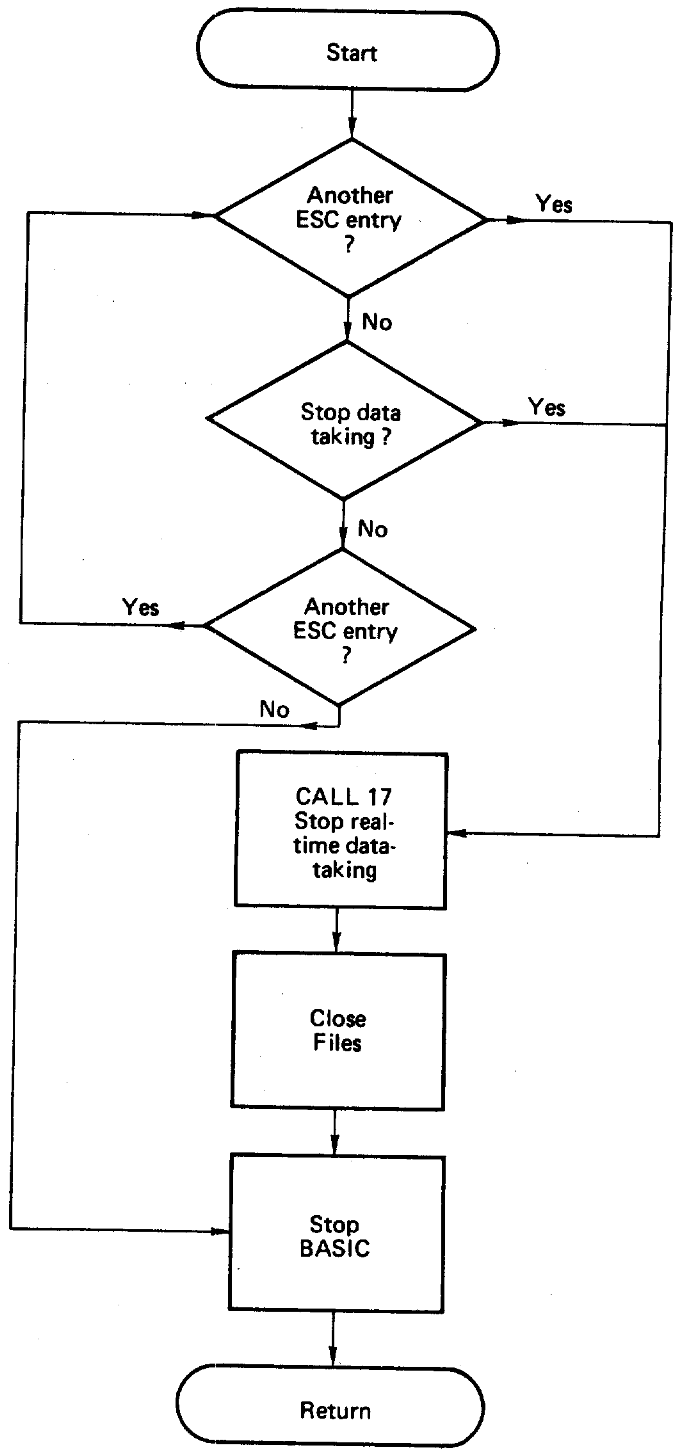

FIG. 7. Logic flow diagram of the subroutine that handles the entry of ESCapes.

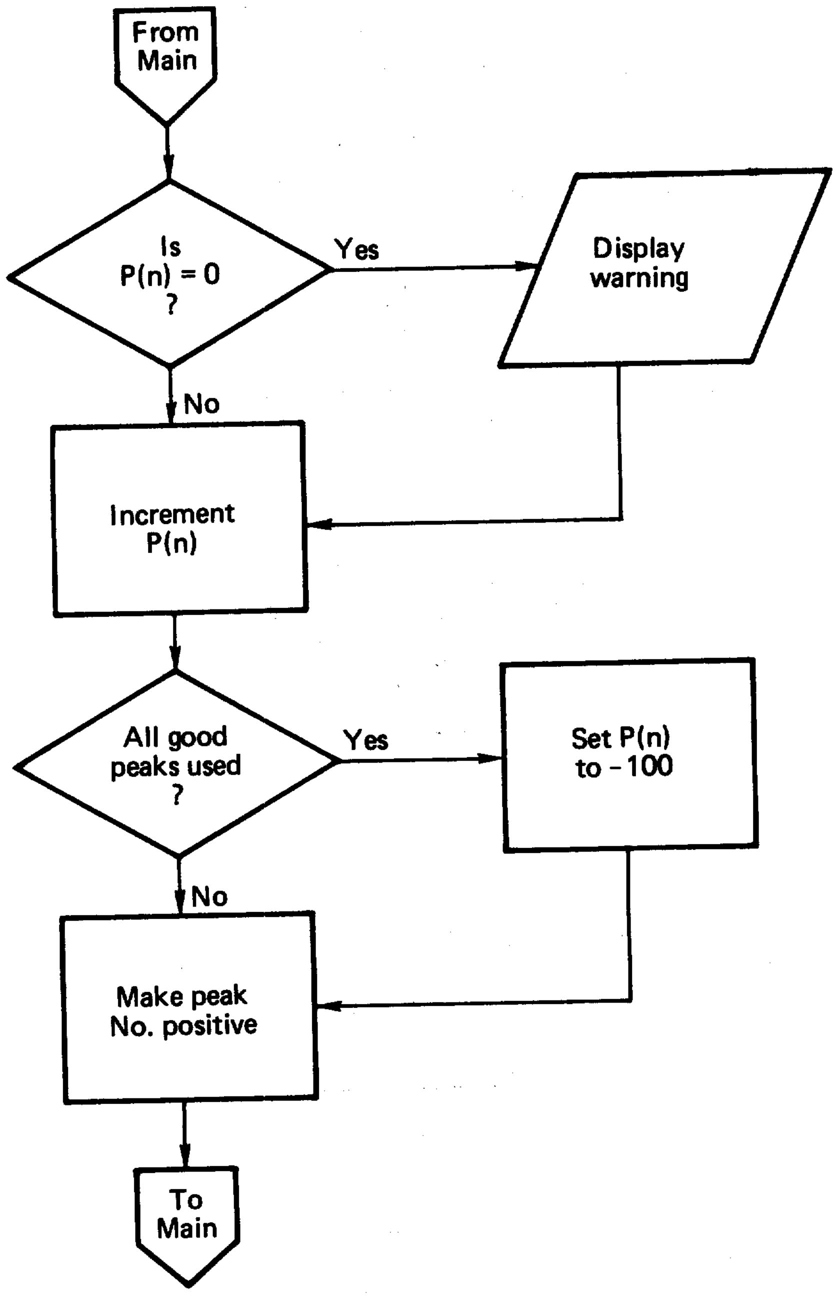

FIG. 8. Logic flow diagram of the subroutine that handles the overflow of the peak-data buffer. P(n) is the number of good peaks left.

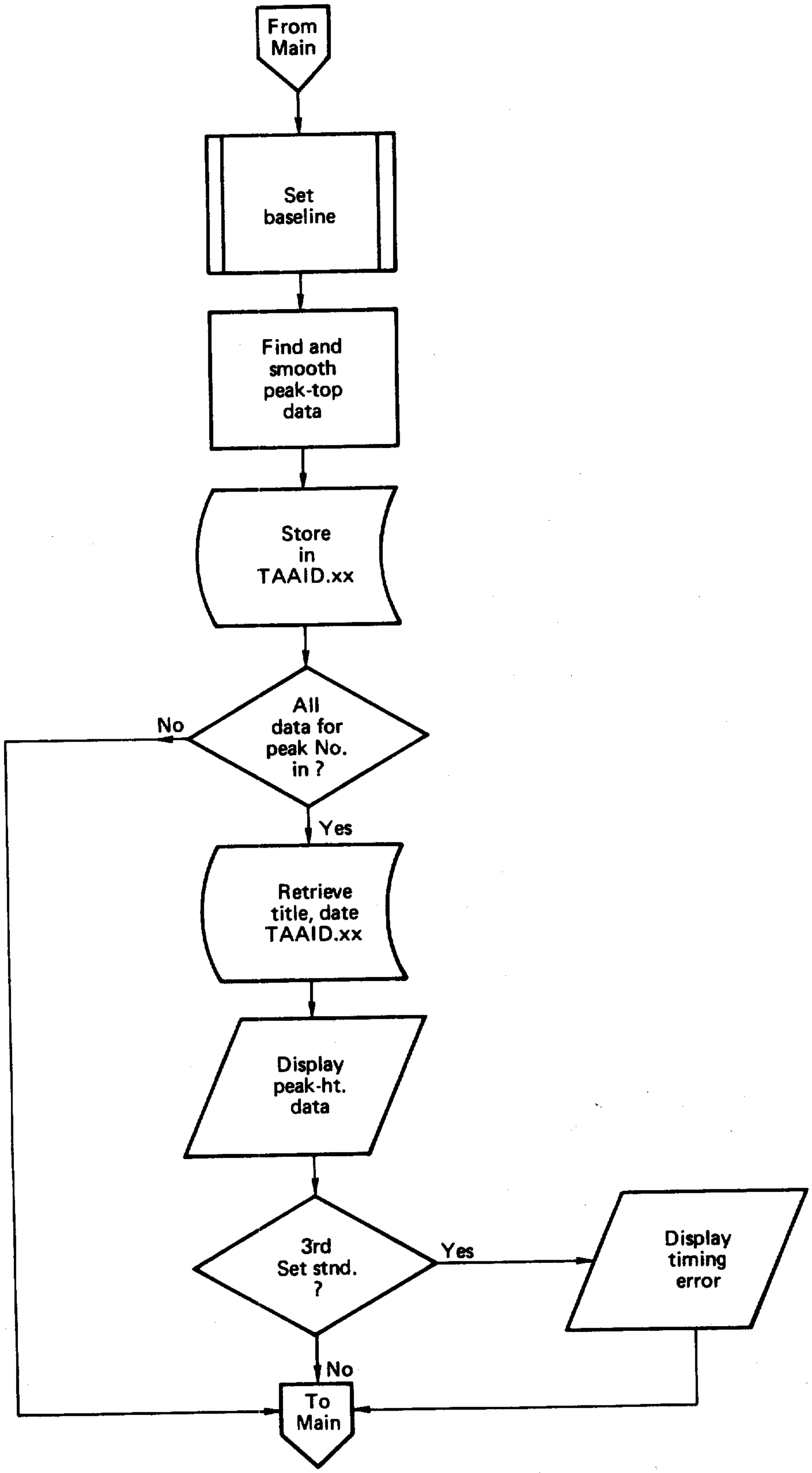

FIG. 9. **Logic flow diagram of the subroutine that processes Set standards.**

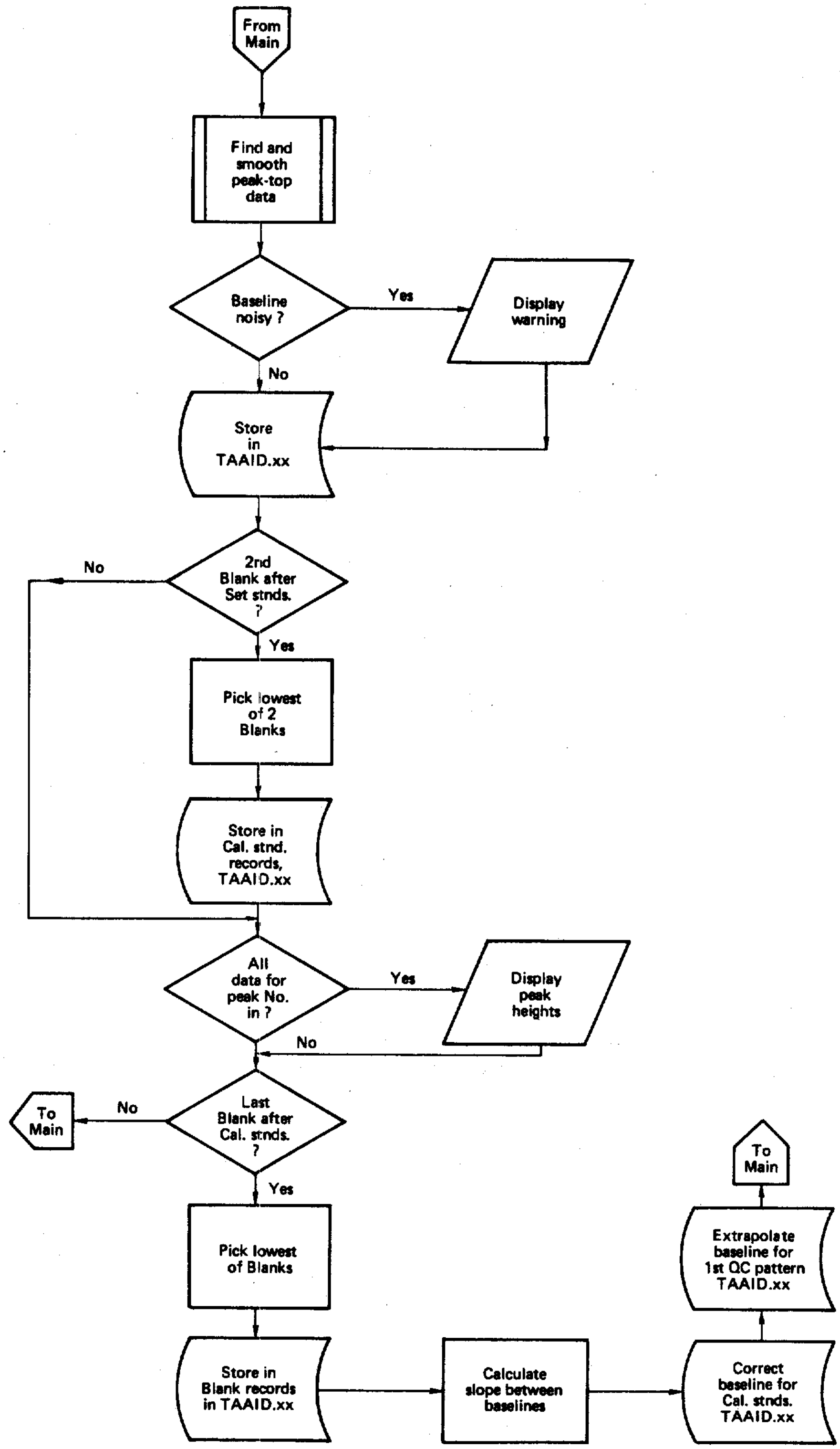

FIG. 10. Logic flow diagram of the subroutine that processes Blanks.

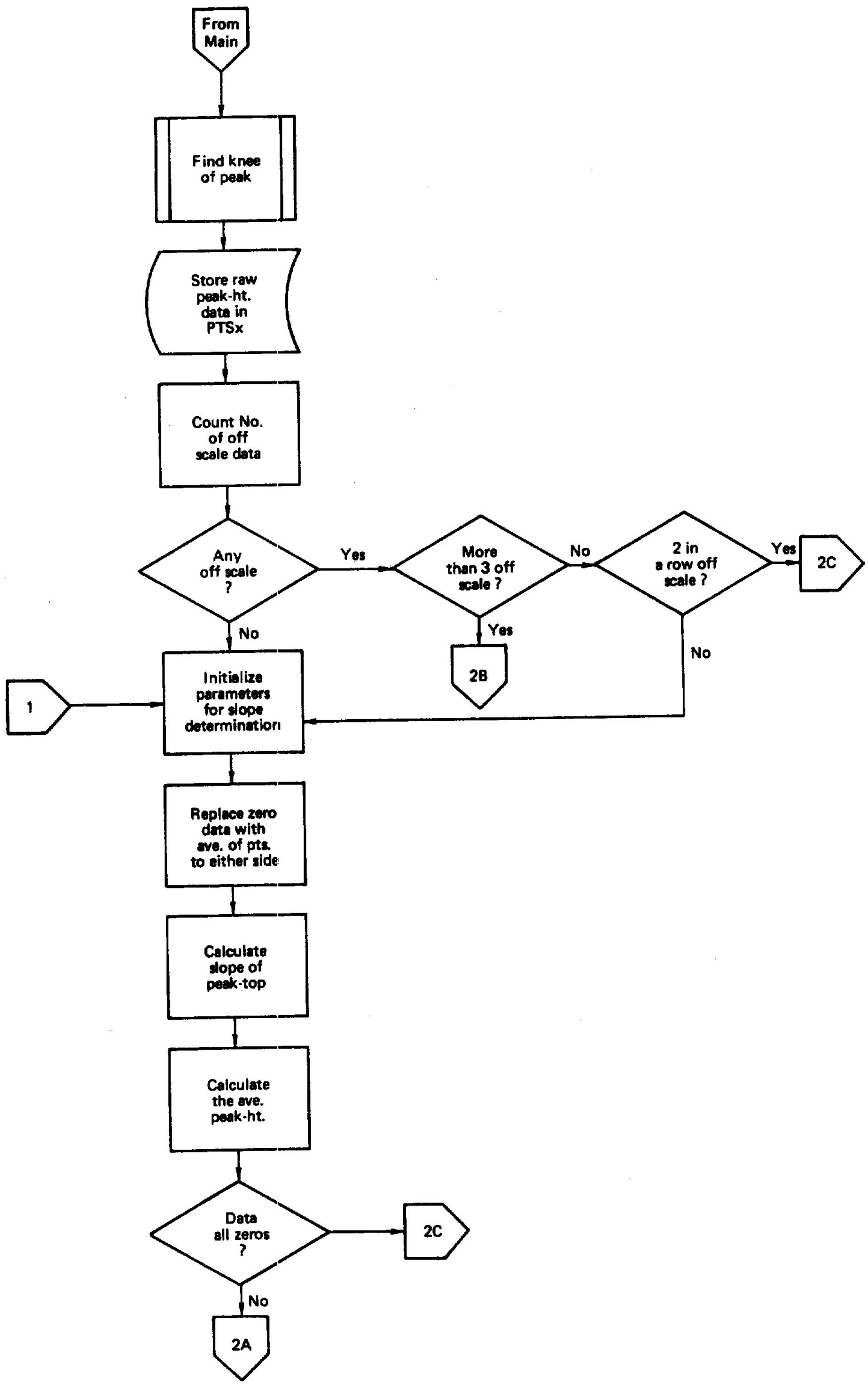

FIG. 11. Logic flow diagram of the subroutine that processes Calibration standards.

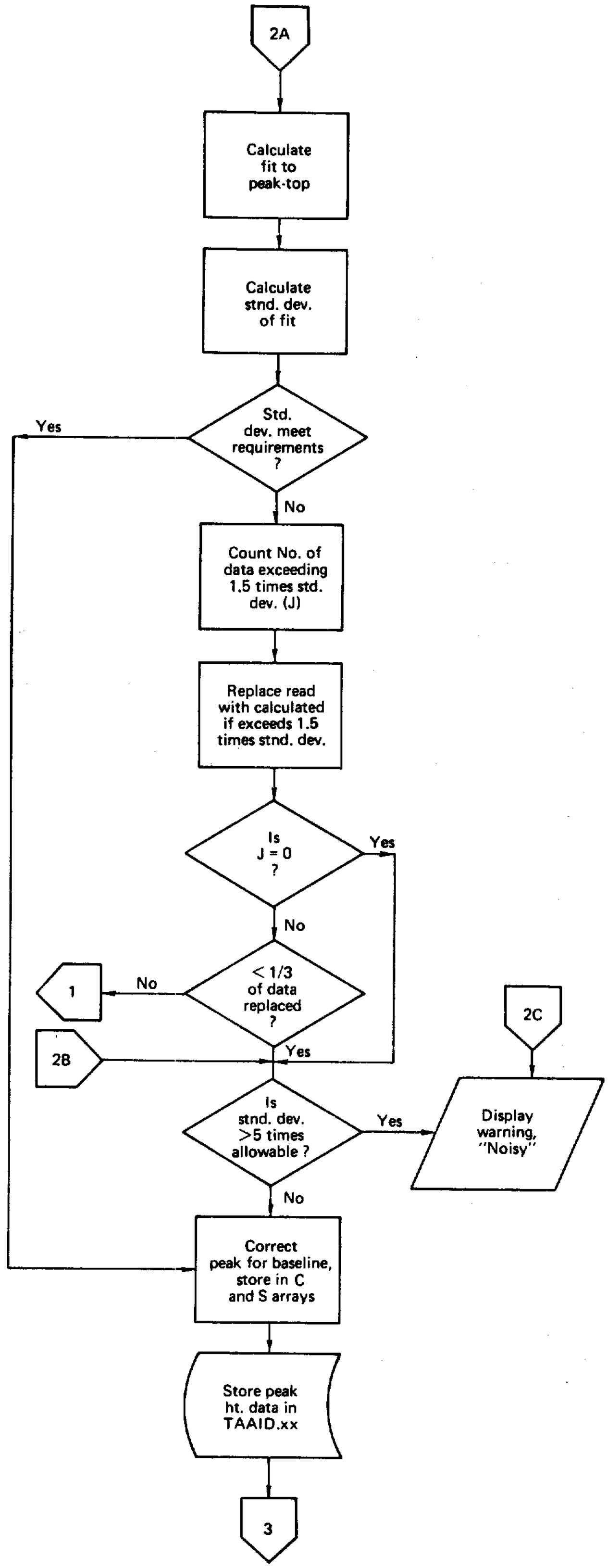

FIG. 11. (Continued.)

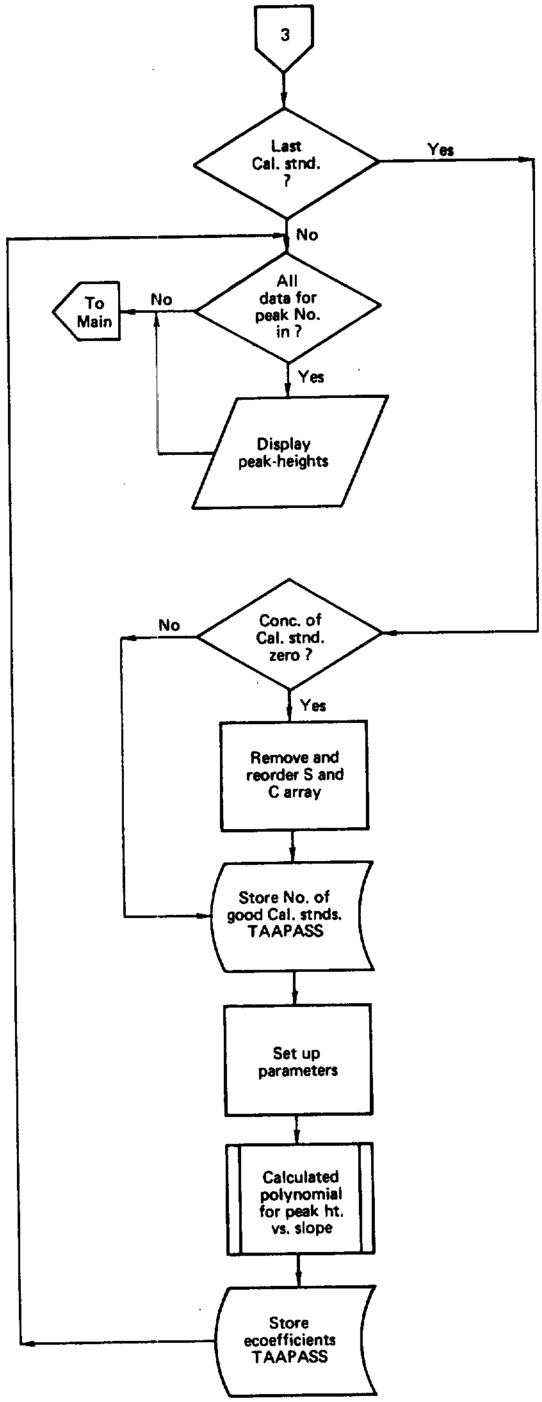

FIG. 11. (Continued.)

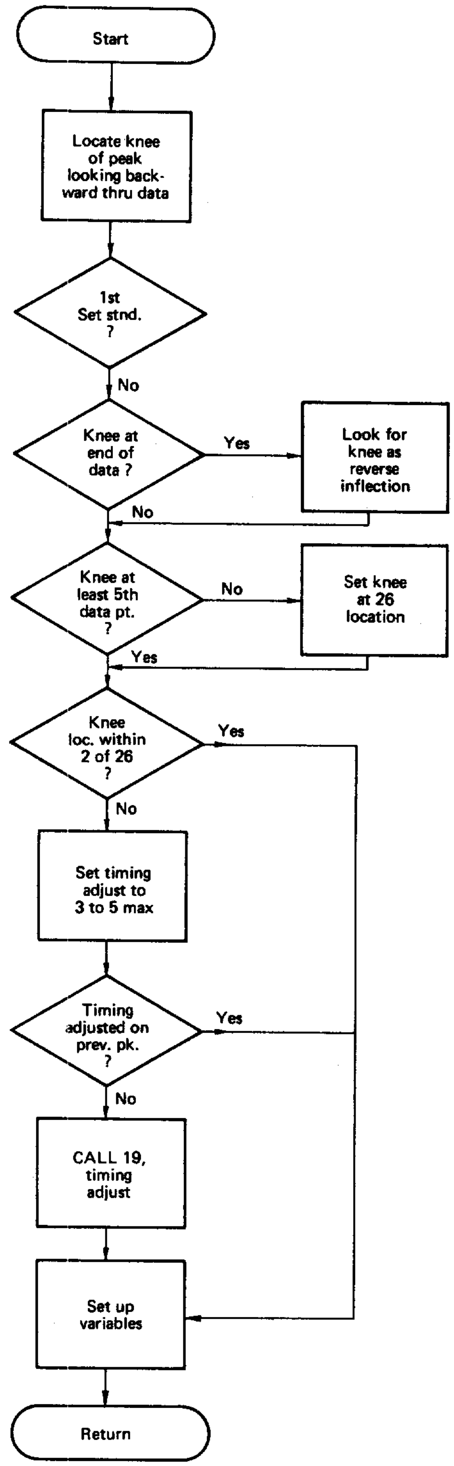

FIG. 12. Logic flow diagram of the subroutine that finds the peak top.

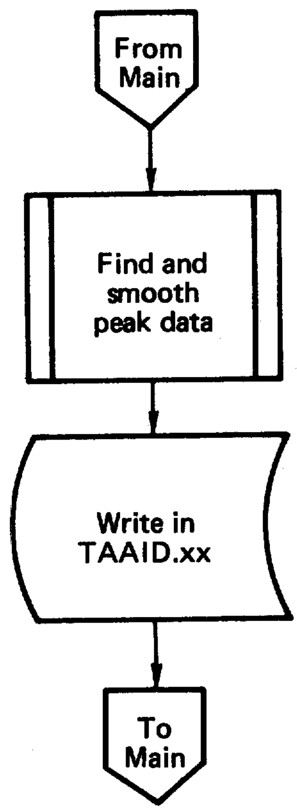

FIG. 13. Logic flow diagram of the subroutine that handles samples and reagent Blanks.

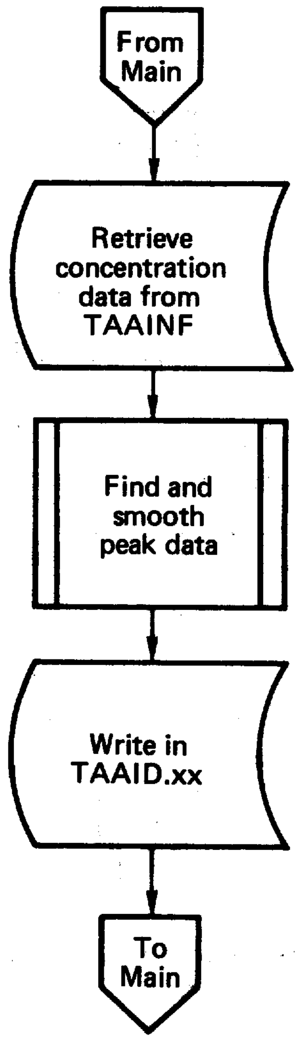

FIG. 14. Logic flow diagram of the subroutine that handles Check standards.

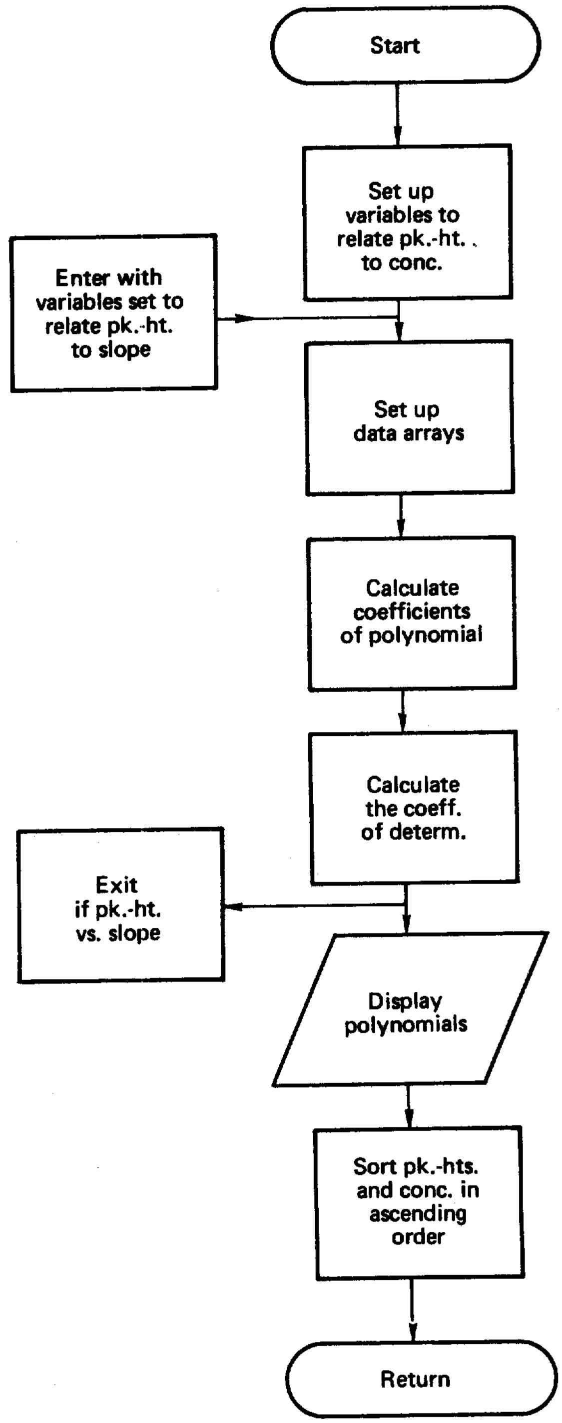

FIG. 15. Logic flow diagram of the subroutine that calculates polynomials and sorts the standards.

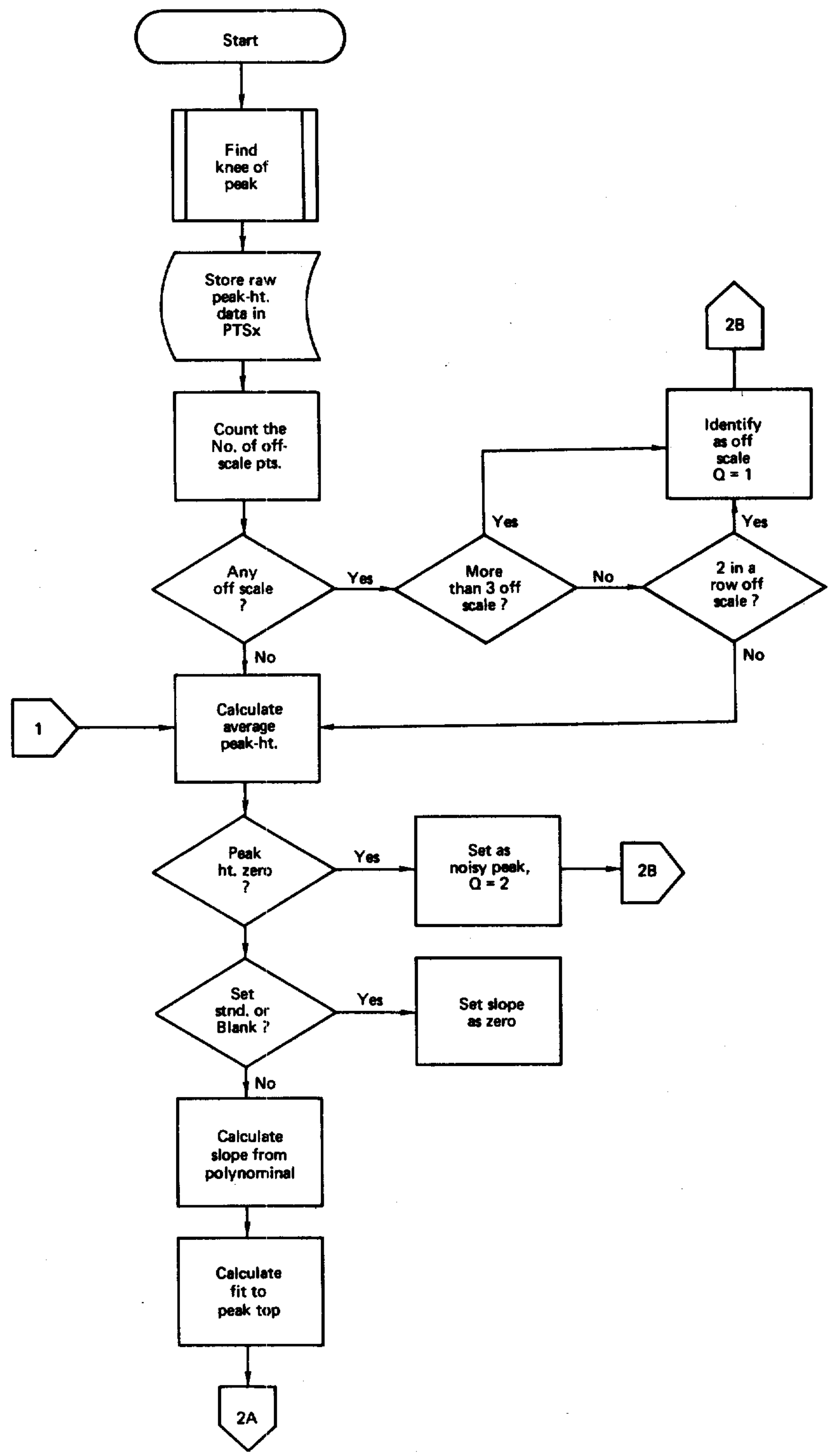

FIG. 16. Logic flow diagram of the subroutine that smooths the data.

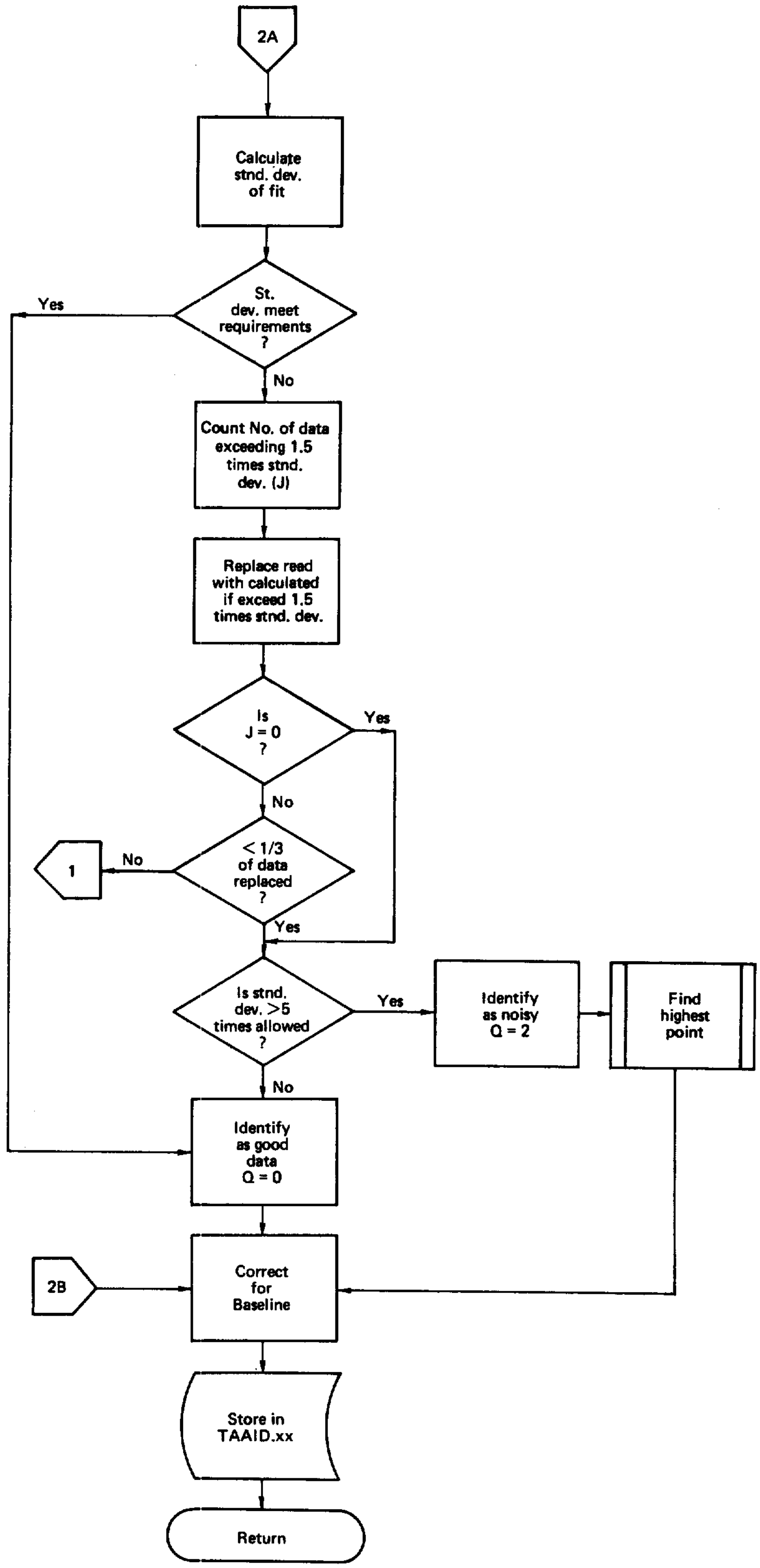

FIG. 16. (Continued.)

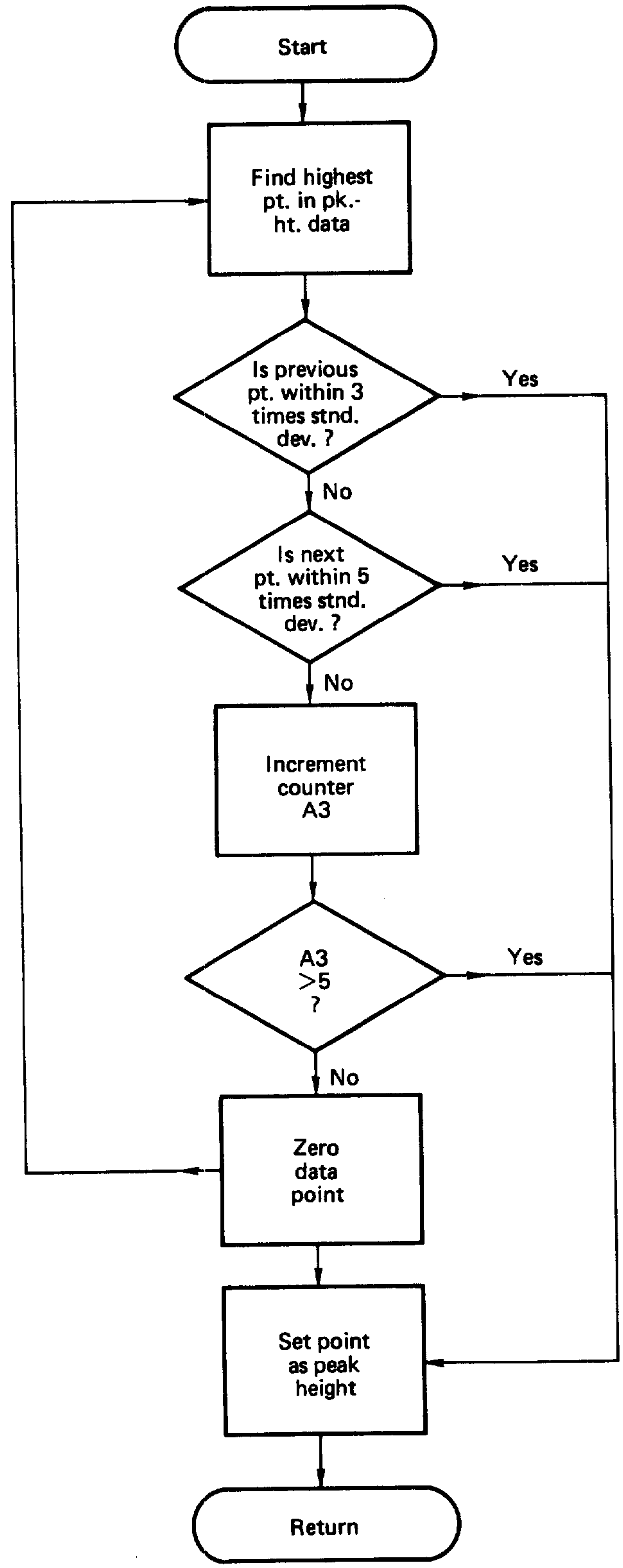

FIG. 17. **Logic flow diagram of the subroutine that finds the highest point in a peak.**

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1. R. W. Crawford, *Computer Automation of Continuous-Flow Analyzers for Trace Constituents in Water*, Lawrence Livermore Laboratory, Livermore, Calif., UCRL-52532, Vol. 4, pt. 1 (1979).
2. L. Taber, H. S. Ames, R. K. Yamauchi, G. W. Barton, Jr., *Instrument Calls and Real-Time Code for Laboratory Automation*, Lawrence Livermore Laboratory, Livermore, Calif., UCRL-52392 (June 7, 1978), p. 84.

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APPENDIX A
PROGRAM SECTIONS AND SUBROUTINES

MAIN PROGRAM

Line Numbers	*Description of Operation*
0050-0145	Dimension arrays, and open files.
0150-0200	Initialize variables, and dimension arrays.
0205	Print analyte names for column headings.
0210-0240	Read peak-height using CALL 18.
0300-0315	Set variables to peak number.
0320	Open appropriate TAAID.xx file and retrieve data for current peak.
0325-0435	Branch to the appropriate peak processing routine based upon the type, T, of the peak.
0440-0470	See if all calibration standards have been measured, or that all peaks have been processed after a peak buffer overflow.
0472-0476	See if there are additional data to be processed.
0478	Allow operator to terminate after a buffer overflow.
0480-0520	Get data for the calibration polynomial.
0540-0620	Store appropriate data in TAAPASS.
0630	CHAIN to program TAA.

SUBROUTINES

Subroutine to Handle Escape

0700	If two ESCapes are hit, kill both the assembly language and the BASIC program.
0710-0840	If one ESCape is hit, find if the operator wants to kill the real-time program. Either way, stop BASIC. This is most useful during debugging.

Subroutine to Handle Overflow of Peak Data Buffer

1000	If the peak data buffer has overflowed, print warning.
1010-1040	Increment the pointer to the remaining good peaks in the buffer.
1050-1060	Set counter to −100 to indicate all good peaks have been processed.
1100-1120	Warning message called at 1000.

Subroutine to Process Set Standards

2600	Set baseline to value set in program TAASTART.
2610	Find and smooth peak top data.
2615-2620	Store data in TAAID.xx.
2630-2650	See if all analytes for this peak number have been completed.
2660-2670	Retrieve title data.
2680-2740	Print peak-height data for all analytes of this peak number.
2750	Return to main program if the first or second Set standard.
2760-2810	Print the timing error between the second and third Set standard; that is, the difference between the value entered in TAAIN and the value actually observed.

Subroutine to Process Blanks

3000	Smooth the data. Note that most Blanks will be indistinguishable from baseline.
3010-3360	Print warning if Blank is noisy.
3370-3390	Store Blank value in the appropriate TAAID.xx record.
3400	If not the second Blank after the three Set standards, jump to 3450.
3402-3409	Pick the lower of the two Blanks.
3410-3440	Write the Blank into the Calibration standard records.
3450-3480	See if data has been recorded for this peak number for all analytes.
3490-3495	Retrieve title data.
3500-3647	Print data for this blank number for all analytes.
3650	If not the last Blank after the Calibration standards, return to the main program.
3670-3690	Write the value of the Blanks after the Set standards into variable M.
3695-3709	Pick the lower of the Blanks after the Calibration standards, store in both Blank records of TAAID.xx and write into variable B.
3710	Calculate the slope between the earlier and later pairs of Blanks.
3717-3770	Correct peak heights of Calibration standards for the calculated baseline and extrapolate the baseline for the next QC pattern.
3780-3790	Return to the main program.

Subroutine to Process Calibrate Standards

4000-4040	Find the knee of the peak top.
4280-4310	Store the peak data array in PTSx (where x is 1 to 3 depending on the analyte number) and count the number off-scale data points.
4320-4330	Jump to 4390 if no off-scale data, 4800 if more than three.
4340-4380	Look for at least two off-scale data in a row; if found, jump to 4805.
4390-4430	Initialize parameters for determining slope.
4440-4470	Examine the 11 or 21 points used in calculating the peak-height. If any zeros are found, replace with the average of the data on either side. Use this data to calculate slope (see UNUSUAL ALGORITHMS, above).
4490-4580	Calculate the average peak height (F1). If the data are all zeros (usually due to a large negative baseline drift), go to 4805.
4590-4660	Calculate the best fit of a straight line to the data, using previously determined slope. Calculate the standard deviation (see UNUSUAL ALGORITHMS, above).
4680	If the standard deviation meets the operator-entered criterion, jump to 4850.
4690-4750	Count the number of data (J), where the difference between the calculated and the observed values is 1.5 times the standard deviation or more. Replace observed data that exceeds this criterion by the calculated value.
4760	If no data meet this criterion, go to 4800.
4765-4780	If fewer than one-third of the observed data have been replaced by calculated values, go back and reprocess, (4430).
4800-4802	If more than one-third of the data points are noisy, (deviate by more than 1.5 times the allowable standard deviation) or the standard deviation is more than five times the allowable, go to 4805, (noisy). Otherwise go to 4850, ("fuzzy" or Gaussian noise).
4805-4840	Print warning that peak is noisy, suggest hitting ESC to stop. Set Q equal to 2, (noisy), and then use a subroutine (9400) that finds the highest point in the data and uses that as the peak-height. Jump to 4880.
4850	If all tests are passed, set Q = 0.
4880-4930	Correct peak-height for baseline. In case of program TAA1CAL, convert % transmission to absorbance. Write the peak-height and concentration data into arrays, and store them in file TAAID.xx.
4940	If all the Cal standards for this analyte have been run, calculate the polynomial that relates peak slope to height.

4950-4980 See if data have been recorded for this peak number for all analytes. If not, return to the main program.

4990-5070 Print peak-height data for this peak number for all analytes. Return to the main program.

5080-5164 Check for any Cal standards with zero concentration. If found, remove. Reorder the C (concentration) and S (peak height) arrays. Store the number of nonzero standards in TAAPASS.

5180-5520 Set up variables preparatory to calculating the quadratic that relates the slope across the peak tops to concentration.

5230 Calculate the quadratic that relates the slope across the peak tops to concentration.

5240-5300 Write the coefficients of above quadratic into the C array and store in TAAPASS, then return to 4950.

Subroutine to Find the Peak Top

5520-5535 Look backwards through the peak data for knee of the peak, the point at which the slope changes from negative to zero. Data must be at least 800 A/D counts above baseline to be considered.

5539 Skip some logic if the peak is the first Set standard, as the data on this peak are frequently poor.

5540 If the knee is the last point in the data array, go to a routine to look for a reverse inflection (5700).

5545-5555 If the knee is located between the 5th and 34th data point, go to the section that checks if timing needs correction (5590). If knee is at the 4th or earlier location (usually because peak is less than 10% of full-scale), set the knee at the 26th location, and go to 5610.

5565-5572 Make a timing correction using CALL 19 if a correction was not made on the previous peak.

5575-5585 Adjust parameters so at least 11 points will be used in finding the peak height; then go to 5610.

5590-5605 The knee location is compared to 26, and a timing correction made if the knee is 3 or more locations to either side.

5610-5620 Set variables and return.

5700-5780 Look for a reverse inflection.

Subroutine to Handle Samples and Reagent Blanks

6000 Find and smooth peak-top data.

6015-6030 Store peak data in appropriate TAAID.xx record and return to main program.

Subroutine to Handle Check Standards

6100-6110 Retrieve Check standard concentration from TAAINF, and write in C4.

6120 Go to the Sample Handling routine, 6000.

Subroutine to Calculate Polynomials and Sort Standards.

The calculation is discussed in more detail in UNUSUAL ALGORITHMS, above.

7000-7300 Calculate the coefficients of the polynomial relating peak-height to concentration (E5 = 1), or slope across the peak-top (E5 = 2). The order of the polynomial is (M - 1). Peak-heights are in the S array, concentrations are in the C(X,1) array, and slopes are in the C(X,2) array.

7310-7390 Calculate the coefficient of determination (goodness of fit) for the polynomial.

7395-7600 Print polynomial and coefficient of determination.

7610-7700 Sort the concentration and peak-height of Cal standards in ascending order using a bubble sort. This makes the interpolation routine easier. Return from subroutine.

Subroutine to Smooth Data

8000-8020 Find the knee of the peak-top.

8180-8220 Store the peak-data array in PTSx (where x is 1 to 3, depending on the analyte number), and count the number of off-scale data points.

8230-8240 Jump to 8400 if no off-scale data, 8820 if more than three.

8250-8390 Look for at least two off-scale data in a row; if found, jump to 8820.

8400-8500 Calculate the average peak-height (F1). If the data are all zeros, go to 8870 with quality set to noisy, (Q = 2).

8501-8510 If smoothing a Set standard or Blank, assume a flat (zero-slope) peak top. Otherwise, calculate the expected slope (F) using the polynomial created from the Cal standards.

8520-8600 Calculate the best fit of a straight line to the peak-height data using the previously determined slope. Calculate the standard deviation; (see UNUSUAL ALGORITHMS, above).

8610 If the standard deviation meets the operator-entered criterion, jump to 8760.

8620-8680 Count the number of data (J) where the difference between the calculated value and the observed value is 1.5 times or more of the standard deviation. Replace the observed data that meets this criteria by the calculated data.

8690 If no data meet this criterion, go to 8730.

8700-8720 If fewer than one-third of the observed data have been replaced with calculated, go back and reprocess (8410).

8730-8732 If more than one-third of the data are noisy (more than 1.5 times the allowable standard deviation) or the standard deviation is more than 5 times the allowable, go to 8735, (noisy). Otherwise, go to 8760, ("fuzzy" or Gaussian noise).

8735-8750 Identify peak as noisy (Q = 2), and use subroutine 9400.

8760 Identify as good data (Q = 0).

8780-8786 Set peak-height as the knee location in the calculated peak-height data. In the case of program TAA1CAL, convert the % transmission to absorbance.

8790-8810 Skip to exit section.

8820-8860 Identify as off-scale (Q = 1). A crude peak-height is calculated, using the number of off-scale points up to a maximum of five times the full scale.

8870-8890 Correct for baseline, store in the appropriate record of TAAID.xx and return.

Subroutine to Find Highest Point in Peak

9400-9420 Locate highest point in data array.

9425-9445 If the highest point is more than five times the allowable standard deviation higher than the point to either side, set it to zero and find the next highest point. Otherwise, identify highest point as peak-height, and return.

Subroutine to Print Column Headings

9500-9560 Display the analyte names in the appropriate place on the terminal to identify peak-height data.

Subroutine to Open and Retrieve from TAAID.xx

9600-9620 Create the file name by concatenating TAAID with the first two letters of the analyte's name.

9630-9650 Open the file, retrieve data from the appropriate record and return.

APPENDIX B
VARIABLES

A — The number of data points that are used to establish the peak-height. Out of the 35 points returned by the real-time code, only A = 11 or 21 are used for peak-height, with the last point being at the knee of the peak. The other points are used to identify the knee, and to provide a margin for error in the timing. The references to A in lines 7300 to 7360 refer to the array A, used in matrix operations.

A2 — The offset to the record number in the wheel patterns. The contents of A2 increment by steps of 300, with A2 = 0 for wheel pattern 1, A2 = 300 for wheel pattern 2, A2 = 600 for wheel pattern 3, and so on.

A3 — A pointer to the current peak in correcting for baseline, for the standards in calculating the calibration polynomial, and for data points in finding the top of a peak.

A5 — The current estimate of the peak-top location.

B — Value of the baseline subtracted from each peak. Initially, it is the lower of the blanks after the set standards. After calculation, it is the value linearly interpolated between the lower blanks before and after the set standards.

C — Used only for reading and writing TAAID.xx records.

C4 — The nominal concentration of a calibration standard, as entered by the operator.

D1 — The allowable standard deviation of the points used to measure the peak-height.

E1 — The number of the record in file TAAID.xx currently being retrieved or stored. It is calculated by adding the number of the peak being processed, B[x], to the offset, A2.

E2 — A scratch variable used to count the raw peak-height data that are off-scale, and in calculating the coefficients of quadratic fits.

E3 — The standard deviation of the data points used to calculate the peak height.

E4 — A scratch variable used in calculating the slopes of peak-tops and the coefficients of quadratics.

E5 — A variable calling out either the first column of the C matrix for peak height vs concentration, or the second for peak slope vs concentration in calculating quadratic fits.

E7 — The coefficient of determination of the peak height and slope equations. It should be as close to 1 as possible.

E8 — A flag used to exit from the slope and height calculations. For concentration, it is 0, for slope, it is 1.

F — The slope across the top of the peak calculated in lines 4430 to 4470, where A is the 11 or 22-point fit, K is the index, Y is the midpoint = (A + 1)/2, D[K] is the peak height datum, and E4 is 110 for 11 points or 770 for 21 points.

F1 — The average peak-height of the 11 or 21 points preceding the knee, excluding noisy data.

F2 — The address of the location of the knee of the current peak, as found in the D array.

F3 — Reserved for an offset pointer to information in TAAINF.

G — See array G.

G1 — The number of peaks that CALL 18 will store on disk.

H — See array H.

H1–H4 — Quality control constants not used in TAACAL, but they must be kept for file reads and writes.

I, J — Counters for loops.

J1 — Used only for file reads and writes.

K — Counter used for loops.

L — From statements 3710 to 3763, this is the slope of the baseline. Elsewhere, it is used in calculating the concentration and slope equations.

M — From statements 3690 to 3763, it is the baseline taken from the lower of the two initial blanks. In lines 4500 to 4660 and 8420 to 8600, it is the sum of the squared difference between measured and calculated peak-height. Elsewhere, it is one more than the order of the fitting polynomial.

M1 — A pointer which finally contains the location of the knee of the peak. R[M1] is the peak height.

M2 — A counter used in locating M1.

N — The analyte number defined by TAAIN.

N0 The total number of analytes in this run.
N1 The number of Calibration standards.
N2 The number of Blanks in a single pattern.
N8 The number of samples and Check standards in a pattern.
N9 The total number of samples and Check standards in this run.
P Position in the sample wheel.
P1 The number of the wheel.
Q The quality-control code, where
- -1 Initialized value
- 0 Good data
- 1 Out of calibrate range or off-scale
- 2 Noisy peak
- 3 Diluted sample OK
- 4 Bad for the second time
- 5 Does not pass quality control
- 6 Fails quality control, and is noisy or off-scale
- 7 Duplicate or spike is being compared to noisy or off-scale sample and fails quality control
- 8 Same as 7, but passes quality control.

R Raw peak-height in A/D units.
S, S1 Used only for File reads and writes.
T Type of sample, where
- 1 Set standard
- 2 Blank
- 3 Calibration standard
- 4 Unknown
- 5 Check standard
- 6 Spike
- 7 Duplicate
- 8 Reagent blank
- 9 End of run.

T0 Original sample dilution factor.
T1 Sample label. For Blanks and Check standards, it is the consecutive number. For Spikes and Duplicates, it is the sample identification number from TAAID.xx.
U, W See Arrays U and W.
X In lines 150 and 180, X is a scratch variable. Elsewhere, X is the peak-height corrected for baseline in A/D units.
X1 The number of data values in the peak-height array that differ from the calculated line by more than 1.5 standard deviations.
Y In lines 3727 to 3730, Y is a counter for subtracting baseline from peak-height. In lines 4410–4620 and 8520–8560, Y is the center point of the peak-height fit. For lines 7030–7320, see array Y.
Y9 The order of the fitting polynomial. If Y9 = 4, interpolation is used.
Z See array Z.

APPENDIX C
ARRAYS

A[x,y] One of the eight arrays used in the matrix calculation of the coefficients of the fitting polynomial that relates concentration, R, to A/D signal, S, as follows:

$$R = a_{1,1} + a_{2,1}s + a_{3,1}s^2 + a_{4,1}s^3$$

B[x,y] The major array that contains constants for each analyte. The analyte number is x.

- B[x,1] Is the sequential peak number. When the program calls for B[x], the interpreter returns B[x,1].
- B[x,2] The number of points used to define peak height, 11 or 22. (See Variable A.)
- B[x,3] The acceptable standard deviation for points across the peak top when calculating height.
- B[x,4] The interval between data points in 2/15-second ticks defined by the operator's response to the TAAIN prompt, "DATA RATE 15 TO 60."
- B[x,5] The A/D channel number.
- B[x,6] The record number of the last calibration standard that needed a timing correction. This is used to avoid making duplicate timing corrections.
- B[x,7] The full-scale reading of the colorimeter in A/D units, divided by 100. This is used to convert readings to percent of full-scale to match chart records.
- B[x,8] The blank or baseline reading of the colorimeter in A/D units.
- B[x,9] The record number of the last blank in the Calibrate pattern.

C[x,y] Information about Calibration standards. If n is the sequential number of each analyte, and T1 is the sequential number of each standard, then

$$C_{1,n+2} \text{ to } C_{3,n+2}$$

are the coefficients of the quadratic relating slopes of the peak tops, S, to peak-height, p:

$$S = C_{1,n+2} + C_{2,n+2}p + C_{3,n+2}p^2$$

$$C_{10(n-1)+T1,\,1}$$

are the concentrations of the calibration standards entered by the operator. Initially they are in the order entered, but just before chaining to TAA, they are sorted in ascending concentration, leaving out any standards that are entered as zero concentration.

$$C_{10(n-1)+T1,\,2}$$

are the slope of the peak-top for each of the standards.

D[x] Contains the most recent raw peak-height data for each analyte—the 35 A/D readings returned to the BASIC program on completion of CALL 18.

E[x] Contains the peak number of the data in D[x] for each analyte in the order entered by the operator.

F[x,y] Stores the locations of the knees of the set standards. Analyte number is x, standard number is y.

G[x,y] Is used in calculating the polynomial fit.

H[x,y] Is used in calculating the polynomial fit.

K[x,y] Is used in calculating the polynomial fit in statements 7360 and 7370.

L[x] Stores the difference between calculated and measured peak heights of the standards.

M[x] Is used with CALL 19, shift timing of data collection where

- M[1] Is the A/D converter channel number.
- M[2] Is the number of 2/15-second ticks by which the sample window timing must be corrected. Because of computing delays, the correction cannot be made before the second succeeding peak. The criterion is that the knee must have drifted to earlier than the 24th or later than the 28th of the 35 data values returned by CALL 18. The correction is limited to 3, 4, or 5 ticks.

P[x] Is a counter and flag used to retrieve peaks from disk storage when core storage has been exceeded. Ordinarily, the real-time program returns data directly to TAACAL. If for any reason the BASIC program does not make a CALL 18 before another peak is ready to be written into the D array, data will be written directly to the disk. This may come about because of heavy competition from other users or because the BASIC program has been stopped by the ESCape key or by an error. As long as the allocated disk space is not exceeded, the BASIC program continues. If storage has been exceeded, CALL 18 returns the negative of the peak number in E[N]. If overflow has occurred, P[x], where x is the analyte number, counts peaks until all available have been read. At that time P[x] is set to -100.

R[x] Is the calculated peak height before baseline correction.

S[x] Is the peak height of Calibration standards in A/D units corrected for baseline. Data are stored in this array in groups of 10. S[1] through S[10] are for the first analyte, S[11] through S[20] for the second, and so on.

U[x,y] Is used in calculating the polynomial fit.

W[x,y] Is used in the polynomial fit.

X[x,y] Is used in the polynomial fit.

Y[x,y] Is used in the polynomial fit.

Z[x,y] Is used in the polynomial fit.

APPENDIX D
STRINGS

A$ Is the name of the analyte, such as Cl, SO_4, or Total Kjeldahl nitrogen (TKN).

B$ Is a string of all the analyte names. Ten characters are set aside for each.

J$ Is a scratch string used for padding with blanks, entering answers to prompts, and opening the correct TAAID.xx file.

Z$ Is used to retrieve strings from files.

APPENDIX E
MODIFICATIONS TO OPERATE THE AUTOANALYZER-I; TAA1CAL

The TAA programs require modification for use with the older AutoAnalyzer-I. They are indicated in the computer system library by the name TAA1CAL instead of TAACAL, and so forth. The important difference in the programs is that the AutoAnalyzer-II output is already converted to absorbance, A, while the AutoAnalyzer-I output is the transmittance, T. Their values are related by Beer's law, as follows:

$$A = \log_{10}(1/T) .$$

In order to keep the BASIC and assembly-language programs as much the same as possible, the output of the colorimeter is reversed and offset so that T = 100% is a signal close to 0 V, while T = 0% is close to the full-scale 10 V. Because of this, the peaks generally look similar, and the timing programs still function.

During the instrument setup, the zero reading is taken with a shutter before the colorimeter, and it is stored in B[N,8]. The full-scale reading is taken with a blank in the colorimeter, and B[N,8] less the full-scale reading is stored in B[N,7]. If R is the reading from an unknown,

$$T = 1 - (R - B[N,8])/B[N,7]$$

This is converted to absorbance at line 4886 of the program. Since Beer's law is stated in common logarithms, and only natural logarithms are available in this BASIC, the formula must read

$$A = -\log(T)/\log(10)$$

That is the source of the factor in the denominator.

S[N,2] is used only in TAA1CAL. It stores the raw A/D peak-height of each Calibration standard used in the polynomial fit.

The two partial listings following show the exact differences between TAA1CAL and TAACAL.

Table 1. Source program differences in TAA1CAL; these lines are in TAA1CAL but not in TAACAL.

```
0010  REM **********TAA1CAL*********
0016  REM MERL VERSION FOR TAA-1
0183  REM
0184  REM
0630  CHAIN "TAA1"
2600  LET B=.0001
2720  PRINT USING "--.####A      ",X;
3560  PRINT USING "--.####A      ",R;
3643  PRINT USING "--.####A *    ",R;
4880  LET R=(B[N,7]-(R[M1]-B[N,8]))/B[N,7]
4881  IF R=0 THEN GOTO 4890
4882  IF R>0 THEN GOTO 4886
4883  LET R=-LOG(-R)/2.30259
4884  LET R=-R
4885  GOTO 4890
4886  LET R=-LOG(R)/2.30259
4890  LET X=R-B
4895  LET S[(N-1)*10+T1,2]=R[M1]
5020  PRINT USING "--.####A      ",S[(I-1)*10+T1];
5145  LET S[(N-1)*10+A3,2]=S[(N-1)*10+K,2]
5195  LET S[(N-1)*10+A3+1,2]=0
5525  IF D[J+(N-1)*35]-B[N,8]<800 THEN GOTO 5535
5710  IF D[35+(N-1)*35]-B[N,8]<800 THEN GOTO 5550
7120  LET X=S[(N-1)*10+I,E5]
8780  IF R[M1]>=B[N,7]+B[N,8] THEN LET R[M1]=(B[N,7]+B[N,8])-.0001
8781  LET R=(B[N,7]-(R[M1]-B[N,8]))/B[N,7]
8786  LET R=-LOG(R)/2.30259
```

Table 2. Source program differences in TAACAL; these lines are in TAACAL but not in TAA1CAL.

```
0010  PRINT "TAACAL 11683 05/27/77 8:38 9660 RC"
0183  LET B[I,7]=B[I,7]/100
0184  REM USED TO PRINT % OF F.S.
0630  CHAIN "TAA"
2600  LET B=B[N,8]
2720  PRINT USING "--##.##%      ",X/B[K,7];
3560  PRINT USING " --#.##%      ",(R-B[I,8])/B[I,7];
3643  PRINT USING " --#.##% *    ",(R-B[I,8])/B[I,7];
4880  LET R=R[M1]
4881  REM
4882  REM
4883  REM
4884  REM
4885  REM
4886  REM
4890  LET X=R-B
4895  REM
5020  PRINT USING "--##.##%      ",S[(I-1)*10+T1]/B[I,7];
5145  REM
5195  REM
5525  IF D[J+(N-1)*35]-B<800 THEN GOTO 5535
5710  IF D[35+(N-1)*35]-B<800 THEN GOTO 5550
7120  LET X=S[(N-1)*10+I]
8780  LET R=R[M1]
8781  REM
8786  REM
```

APPENDIX F
PROGRAM LISTING

```
0010 PRINT "TAACAL 11683 05/27/77 8:38 9660 RC"
0015 REM ***** 28-FEB-80 *****
0020 REM CALIBRATE PROGRAM FOR TECHNICON AUTOANALYZER
0030 REM WRITTEN 8/11/75 AT LLL
0040 REM ASSEMBLY PROGRAM - HENRY AMES, BASIC PROGRAM - RICHARD
     CRAWFORD
0050 DIM A[4,4]
0060 DIM G[4,4],H[4,4],K[4,4],L[22]
0070 DIM R[22],W[4,4],Y[10,1],Z[4,4]
0077 LET G1=3
0078 REM NO. OF PEAKS ON DATA DISC
0080 DIM A$[15],J$[20],Z$[1]
0100 DIM E[3],U[4,4],M[2]
0103 LET N=1
0105 ON ESC THEN GOSUB 0700
0110 CLOSE
0111 OPEN FILE[4,1],"PTS1"
0112 OPEN FILE[5,1],"PTS2"
0113 OPEN FILE[6,1],"PTS3"
0114 CLOSE
0115 OPEN FILE[4,2],"PTS1"
0120 OPEN FILE[5,2],"PTS2"
0130 OPEN FILE[6,2],"PTS3"
0140 OPEN FILE[2,0],"TAAINF"
0142 OPEN FILE[3,0],"TAAPASS"
0144 READ FILE[3,8],A2,F3
0145 CLOSE FILE[3]
0150 READ FILE[2,6+F3],N0,N1,N2,X,X,X,X,X,N8,N9
0155 DIM C[N0*10,8],D[N0*35],B$[10*N0],B[N0,9]
0156 DIM F[N0,3],P[N0]
0157 DIM S[N0*10,2]
0160 LET J$="          "
0170 FOR I=1 TO N0
0173   LET E[I]=0
0174   LET P[I]=0
0176   LET B[I,6]=0
0180   READ FILE[2,10+I+F3],A$,B[I,5],Z$,X,X,Z$,J,B[I,2],X,B[I,
          3],B[I,7],B[I,8]
0183   LET B[I,7]=B[I,7]/100
0184   REM USED TO PRINT % OF F.S.
0185   LET B[I,4]=INT(450/J+.5)
0190   LET B$[10*(I-1)+1,10*I]=A$,J$
0200 NEXT I
0205 GOSUB 9500
0206 REM PRINT HEADINGS
0210 LET E[N]=0
0211 REM LOOK FOR A PEAK, ANALYT # IS N
0215 FOR N=1 TO N0
0220   IF E[N]>0 THEN GOTO 0300
```

```
0225   IF E[N]<0 THEN GOTO 1000
0230 NEXT N
0235 CALL 18,E[1],D[1]
0240 GOTO 0215
0300 LET K=N
0312 LET B[N]=E[N]
0315 LET E1=A2+B[N]
0320 GOSUB 9600
0325 IF T=1 THEN GOTO 2600
0326 REM HANDLE SET STAND.
0330 IF T=2 THEN GOTO 3000
0340 REM HANDLE BLANKS
0350 IF T=3 THEN GOTO 4000
0360 REM HANDLE CAL STANDARDS
0370 IF T=4 THEN GOTO 6000
0380 REM HANDLE SAMPLES
0390 IF T=5 THEN GOTO 6100
0400 REM HANDLE CHECK STANDARDS
0403 IF T=6 THEN GOTO 6000
0405 REM HANDLE REAGENT BLANK
0410 PRINT "A TYPE";T;"FOUND FOR ";A$;" AT RECORD";E1
0420 REM A BAD TYPE NO. ENCOUNTERED
0430 STOP
0435 CLOSE FILE[0]
0440 FOR I=1 TO N0
0445   IF P[I]<0 THEN GOTO 0470
0450   IF B[I]<5+N1+N2 THEN GOTO 0210
0460   REM SEE IF CALIBRATION FINISHED
0470 NEXT I
0471 LET E[N]=0
0472 FOR N=1 TO N0
0474   IF E[N]>0 THEN GOTO 0300
0476 NEXT N
0478 IF P[N]<0 THEN GOTO 0710
0480 FOR N=1 TO N0
0485   LET A$=B$[10*(N-1)+1,10*N]
0490   READ FILE[2,20+N],Y9,H1,H2,H3,H4
0500   GOSUB 7000
0510   REM CALCULATE EQUATIONS FOR CONCENTRATION
0520 NEXT N
0540 OPEN FILE[3,0],"TAAPASS"
0550 FOR N=1 TO N0
0560   WRITE FILE[3,N],B[N]
0590   FOR J=1 TO C[5,N+2]
0600     WRITE FILE[3,N*10+J],C[(N-1)*10+J],S[(N-1)*10+J]
0602     WRITE FILE[3,80+N],B[N,9]
0605   NEXT J
0610 NEXT N
0620 CLOSE
0630 CHAIN "TAA"
0699 REM *******SUBROUTINE TO HANDLE ESC ********
0700 ON ESC THEN GOTO 0800
0710 PRINT "DO YOU WANT TO STOP DATA TAKING ";
0720 INPUT J$
0730 IF J$="Y" THEN GOTO 0800
```

```
0740 ON ESC THEN GOSUB 0700
0760 GOTO 0830
0800 CALL 17
0820 CLOSE
0830 STOP
0840 RETURN
1000 LET P[N]=0
1010 LET P[N]=P[N]+1
1020 IF P[N]=G1 THEN GOTO 1050
1030 LET E[N]=ABS(E[N])
1040 GOTO 0300
1050 LET P[N]=-100
1055 LET E[N]=ABS(E[N])
1060 GOTO 0300
1100 PRINT "<7>DATA DISC BUFFER FILLED, NEXT";G1;" PEAKS ARE THE
     ONLY "
1110 PRINT "REMAINING DATA"
1120 GOTO 1010
2595 REM *********** ROUTINE TO HANDLE SET STANDARDS********
2600 LET B=B[N,8]
2610 GOSUB 8000
2615 LET E1=A2+B[N]
2620 WRITE FILE[0,E1],T,Q,P1,P,T1,T0,C4,S,S1,B,R,X,C,E3,J1
2630 FOR I=1 TO N0
2640   IF B[I]<B[N] THEN GOTO 0435
2650 NEXT I
2660 READ FILE[0,E1],T,Q,P1,P
2670 CLOSE FILE[0]
2680 PRINT E1; TAB(5);P1; TAB(7);P; TAB(9);"SET STND";B[N]; TAB(28);
2690 FOR K=1 TO N0
2700   GOSUB 9600
2710   CLOSE FILE[0]
2720   PRINT USING "--##.##%       ",X/B[K,7];
2730 NEXT K
2740 PRINT
2750 IF B[N]<>3 THEN GOTO 0440
2760 PRINT  TAB(4);"TIMING ERROR, SECS."; TAB(28);
2770 FOR K=1 TO N0
2780   PRINT USING "--##.#         ",(F[K,B[N]-1]-F[K,B[N]])*(B[K,
          4]/7.5);
2790 NEXT K
2800 PRINT
2810 GOTO 0440
2995 REM****SUBROUTINE TO HANDLE BLANKS******
3000 GOSUB 8000
3001 REM SMOOTH DATA
3010 IF Q=0 THEN GOTO 3370
3360 PRINT "NOISY BASELINE ON ";A$;" CHANNEL";"<7>"
3370 LET B=R
3385 LET E1=A2+B[N]
3390 WRITE FILE[0,E1],T,Q,P1,P,T1,T0,C4,S,S1,B,B,0,0,E3
3400 IF B[N]<>5 THEN GOTO 3450
3402 READ FILE[0,E1-1],T,Q,P1,P,T1,T0,C4,S,S1,X
3404 IF X>=B THEN GOTO 3410
```

```
3406 READ FILE[0,E1],T,Q,P1,P,T1,T0,C4,S,S1
3408 WRITE FILE[0,E1],T,Q,P1,P,T1,T0,C4,S,S1,X,B,0,0,E3
3409 LET B=X
3410 FOR I=6 TO 5+N1
3415   READ FILE[0,A2+I],T,Q,P1,P,T1,T0,C4,S,S1
3420   WRITE FILE[0,A2+I],T,Q,P1,P,T1,T0,C4,S,S1,B
3430   REM PROJECT BLANK TO USE WITH CAL STNDS.
3440 NEXT I
3450 FOR I=1 TO N0
3460   IF B[I]<B[N] THEN GOTO 3650
3470   REM SEE IF ALL ANALYTS ON THIS BLANK DONE
3480 NEXT I
3490 READ FILE[0,E1],T,Q,P1,P,T1
3495 CLOSE FILE[0]
3500 PRINT E1; TAB(5);P1; TAB(7);P; TAB(9);"BLANK";T1; TAB(28);
3510 FOR I=1 TO N0
3520   LET K=I
3530   GOSUB 9600
3550   IF Q=2 THEN GOTO 3643
3560   PRINT USING " --#.##%      ",(R-B[I,8])/B[I,7];
3630   WRITE FILE[0,E1],T,Q,P1,P,T1,T0,C4,S,S1,B,R,X,C,E3,J1
3632   IF I=N0 THEN GOTO 3640
3635   CLOSE FILE[0]
3640 NEXT I
3641 PRINT
3642 GOTO 3650
3643 PRINT USING " --#.##% *    ",(R-B[I,8])/B[I,7];
3647 GOTO 3630
3650 IF B[N]<>5+N1+N2 THEN GOTO 0435
3660 REM SEE IF LAST BLANK AFTER CAL STDS.
3670 LET A$=B$[10*(N-1)+1,10*N]
3672 CLOSE FILE[0]
3674 LET J$="TAAID."
3678 LET J$=J$,A$
3680 OPEN FILE[0,0],J$
3690 READ FILE[0,A2+5],T,Q,P1,P,T1,T0,C4,S,S1,M
3695 LET E1=A2+B[N]
3700 READ FILE[0,E1],T,Q,P1,P,T1,T0,C4,S,S1,B
3701 IF N2<2 THEN GOTO 3710
3702 READ FILE[0,E1-1],T,Q,P1,P,T1,T0,C4,S,S1,X
3704 IF X>=B THEN GOTO 3710
3706 READ FILE[0,E1],T,Q,P1,P,T1,T0,C4,S,S1,B,B,B,C,E3,J1
3708 WRITE FILE[0,E1],T,Q,P1,P,T1,T0,C4,S,S1,X,B,0,0,E3,J1
3709 LET B=X
3710 LET L=(B-M)/(B[N]-5)
3715 REM SLOPE BETWEEN BLANKS
3717 LET B[N,9]=E1
3720 LET J=0
3725 LET A3=0
3726 IF N9>5+N1+N8 THEN GOTO 3729
3727 LET Y=N9
3728 GOTO 3730
3729 LET Y=5+N1+N8
3730 FOR I=6 TO Y
3740   LET J=J+1
```

```
3750    READ FILE[0,A2+I],T,Q,P1,P,T1,T0,C4,S,S1,B,R,X,C,E3,J1
3755    IF T=2 THEN GOTO 3770
3756    IF T<>3 THEN GOTO 3759
3757    IF X=0 THEN GOTO 3770
3759    WRITE FILE[0,A2+I],T,Q,P1,P,T1,T0,C4,S,S1,L*J+M,R,R-(L*J+M),
           C,E3,J1
3760    IF T<>3 THEN GOTO 3770
3762    LET A3=A3+1
3763    LET S[(N-1)*10+A3]=R-(L*J+M)
3765    REM CORRECT BLANKS FOR DRIFT
3770 NEXT I
3780 LET T=2
3790 GOTO 0435
3995 REM****SUBROUTINE TO HANDLE CAL STANDARDS*******
4000 LET A=B[N,2]
4010 LET D1=B[N,3]
4015 LET E1=A2+B[N]
4040 GOSUB 5520
4280 LET E2=0
4285 FOR K=(N-1)*35+1 TO (N-1)*35+35
4287   PRINT FILE[3+N],D[K]
4290   IF D[K]<16383 THEN GOTO 4310
4300   LET E2=E2+1
4310 NEXT K
4320 IF E2=0 THEN GOTO 4390
4330 IF E2>3 THEN GOTO 4800
4340 FOR K=(N-1)*35+1 TO (N-1)*35+35
4350   IF D[K]>=16383 THEN GOTO 4380
4360   REM LOOKING FOR 2 OR MORE OFF-SCALE IN ROW
4370 NEXT K
4380 IF D[K+1]>=16383 THEN GOTO 4805
4390 IF A=21 THEN LET E4=770
4400 IF A=11 THEN LET E4=110
4410 IF A=21 THEN LET Y=F2-12
4420 IF A=11 THEN LET Y=F2-7
4425 LET X=0
4430 LET F=0
4440 FOR K=F2-A-1 TO F2-2
4445    IF D[K]<1 THEN LET D[K]=(D[K-1]+D[K+1])/2
4450    LET F=F+(K-Y)*D[K]
4460 NEXT K
4462 IF F>0 THEN GOTO 4470
4464 LET F=1
4470 LET C[(N-1)*10+T1,2]=F/E4
4490 LET F1=0
4500 LET M=0
4510 LET J=0
4530 FOR K=F2-A-1 TO F2-2
4540    IF D[K]<1 THEN GOTO 4570
4550    LET F1=D[K]+F1
4560    LET J=J+1
4570 NEXT K
4571 IF F1>0 THEN GOTO 4580
4572 LET R[M1]=0
4573 LET E3=0
```

```
4574 GOTO 4805
4580 LET F1=F1/J
4590 LET F=C[(N-1)*10+T1,2]
4595 LET M1=0
4600 FOR K=F2-A-1 TO F2-2
4605   IF D[K]<1 THEN LET D[K]=F1
4610   LET M1=M1+1
4620   LET R[M1]=(K-Y)*F+F1
4630   LET L[M1]=D[K]-R[M1]
4640   LET M=M+L[M1]^2
4650 NEXT K
4660 LET E3=SQR(M/(J-2))
4680 IF E3<=D1 THEN GOTO 4850
4690 LET J=0
4695 LET M1=0
4700 FOR K=F2-A-1 TO F2-2
4710   LET M1=M1+1
4720   IF ABS(L[M1])<=1.5*E3 THEN GOTO 4750
4730   LET D[K]=R[M1]
4740   LET J=J+1
4750 NEXT K
4760 IF J=0 THEN GOTO 4800
4765 LET X=X+J
4770 IF X>INT(A/3+.5) THEN GOTO 4800
4780 GOTO 4430
4790 REM RECALCULATE SLOPE AND INTERCEPT
4800 IF X<>0 THEN GOTO 4805
4801 IF E3>5*D1 THEN GOTO 4805
4802 GOTO 4850
4803 REM SCATTER NOISE, NO BIG SPIKES
4805 PRINT "CAL STND NO.";T1;"ON ";A$;" CHANNEL IS NOISY","<7>"
4810 PRINT "HIT ESC TO RESTART","<7>"
4820 LET Q=2
4835 GOSUB 9400
4840 GOTO 4880
4850 LET Q=0
4860 REM GOOD DATA
4880 LET R=R[M1]
4881 REM
4882 REM
4883 REM
4884 REM
4885 REM
4886 REM
4890 LET X=R-B
4895 REM
4900 LET S[(N-1)*10+T1]=X
4910 LET C[(N-1)*10+T1]=C4
4920 LET E1=A2+B[N]
4930 WRITE FILE[0,E1],T,Q,P1,P,T1,T0,C4,S,S1,B,R,X,C,E3,J1
4940 IF T1=N1 THEN GOTO 5080
4950 FOR I=1 TO N0
4960   IF B[I]<B[N] THEN GOTO 0435
4970   REM SEE IF READY TO PRINT
4980 NEXT I
```

```
4990 PRINT A2+B[N]; TAB(5);P1; TAB(7);P; TAB(9);"CAL STND";T1;
     TAB(28);
5000 FOR I=1 TO N0
5010   IF S[(I-1)*10+T1]=0 THEN GOTO 5060
5020   PRINT USING "--##.##%        ",S[(I-1)*10+T1]/B[I,7];
5030 NEXT I
5040 PRINT
5050 GOTO 0435
5060 PRINT "        *        ";
5070 GOTO 5030
5080 LET A3=0
5085 FOR K=1 TO N1
5090   REM CALCULATE SLOPE COEFFICIENTS
5100   IF C[(N-1)*10+K]=0 THEN GOTO 5152
5110   LET A3=A3+1
5130   LET C[(N-1)*10+A3,2]=C[(N-1)*10+K,2]
5140   LET S[(N-1)*10+A3]=S[(N-1)*10+K]
5145   REM
5150   LET C[(N-1)*10+A3]=C[(N-1)*10+K]
5152 NEXT K
5153 OPEN FILE[3,0],"TAAPASS"
5154 WRITE FILE[3,70+N],A3
5155 CLOSE FILE[3]
5161 IF A3>0 THEN GOTO 5180
5162 PRINT "NO ACCEPTABLE STANDARDS ON ";A$;" CHANNEL";"<7>"
5164 GOTO 4950
5180 LET C[5,N+2]=A3
5190 LET C[(N-1)*10+A3+1]=0
5192 LET C[(N-1)*10+A3+1,2]=0
5194 LET S[(N-1)*10+A3+1]=0
5195 REM
5200 LET E5=2
5210 LET E8=1
5220 LET M=3
5230 GOTO 7025
5240 LET C[1,N+2]=A[1,1]
5250 LET C[2,N+2]=A[2,1]
5260 LET C[3,N+2]=A[3,1]
5265 LET C[4,N+2]=E7
5266 OPEN FILE[3,0],"TAAPASS"
5267 WRITE FILE[3,N*10],A[1,1],A[2,1],A[3,1]
5268 CLOSE FILE[3]
5300 GOTO 4950
5495 REM**********SUBROUTINE TO FIND PEAK TOP**************

5520 FOR J=35 TO 4 STEP -1
5522   IF T=2 THEN GOTO 5700
5525   IF D[J+(N-1)*35]-B<800 THEN GOTO 5535
5530   IF D[J+(N-1)*35]+15<D[J+(N-1)*35-1] THEN GOTO 5535
5531   IF D[J+(N-1)*35]+25<D[J+(N-1)*35-2] THEN GOTO 5535
5532   IF D[J+(N-1)*35]+30<D[J+(N-1)*35-3] THEN GOTO 5535
5533   GOTO 5539
5535 NEXT J
5539 IF B[N]=1 THEN GOTO 5575
5540 IF J=35 THEN GOTO 5700
```

```
5545 IF J>4 THEN GOTO 5590
5550 LET J=26
5555 GOTO 5610
5565 LET M[1]=B[N,5]
5568 IF E1-B[N,6]<2 THEN GOTO 5575
5570 CALL 19,M[1]
5572 LET B[N,6]=E1
5575 IF J<13 THEN LET J=13
5580 IF J<A+2 THEN LET A=11
5585 GOTO 5610
5590 IF ABS(J-26)<3 THEN GOTO 5610
5600 IF ABS(J-26)<=5 THEN GOTO 5603
5601 LET M[2]=SGN(J-26)*5*B[N,4]
5602 GOTO 5565
5603 LET M[2]=(J-26)*B[N,4]
5605 GOTO 5565
5610 LET F2=(N-1)*35+J
5612 IF B[N]>3 THEN GOTO 5620
5613 LET F[N,B[N]]=J
5620 RETURN
5700 IF D[35+(N-1)*35]<1.05*D[20+(N-1)*35] THEN GOTO 5550
5701 REM SEE IF LAST PT. 5% LARGER THAN MID PT.
5702 REM IF IT IS, LOOK FOR REVERSE INFLECTION
5710 IF D[35+(N-1)*35]-B<800 THEN GOTO 5550
5720 FOR J=35 TO 4 STEP -1
5730   IF D[J+(N-1)*35]-15>D[J+(N-1)*35-1] THEN GOTO 5770
5740   IF D[J+(N-1)*35]-25>D[J+(N-1)*35-2] THEN GOTO 5770
5750   IF D[J+(N-1)*35]-30>D[J+(N-1)*35-3] THEN GOTO 5770
5760   GOTO 5575
5770 NEXT J
5780 GOTO 5545
5995 REM******SUBROUTINE TO HANDLE SAMPLES*********
6000 GOSUB 8000
6010 REM SMOOTHING ROUTINE
6015 LET E1=A2+B[N]
6020 WRITE FILE[0,E1],T,Q,P1,P,T1,T0,C4,S,S1,B,R,X,E3,J1
6030 GOTO 0435
6100 READ FILE[2,F3+30+N],L[1],L[2],L[3],L[4],L[5],L[6],L[7],L[8],
        L[9],L[10]
6110 LET C4=L[T1]
6120 GOTO 6000
6121 REM FOR CHK STND
6990 REM*****SUBROUTINE TO DO 1ST, 2ND, AND 3RD DEGREE
6991 REM FITS.  INPUT A/D IS IN S((N-1)*10+I), CONC. OF
6992 REM EACH STD. IN C((N-1)*10+I).  ORDER OF
6993 REM FIT IN Y9, NUMBER OF VALID STANDARDS
6994 REM IN C(5,N+2),M IS DEGREE OF FIT +1.
7000 LET M=Y9+1
7005 IF M>4 THEN GOTO 7610
7015 LET E5=1
7020 LET E8=0
7025 LET X=C[5,N+2]+1
7030 MAT Y=ZER[X]
7040 FOR I=1 TO C[5,N+2]+1
7050   LET Y[I,1]=C[(N-1)*10+I,E5]
```

```
7060 NEXT I
7070 MAT U=ZER[M,M]
7080 MAT G=ZER[M]
7090 MAT H=ZER[M]
7100 FOR I=1 TO C[5,N+2]+1
7110   LET L=1
7120   LET X=S[(N-1)*10+I]
7130   LET Y=C[(N-1)*10+I,E5]
7140   FOR J=1 TO 2*M-1
7150     IF J>M THEN GOTO 7190
7160     LET U[1,J]=U[1,J]+L
7170     LET H[J,1]=H[J,1]+Y
7180     GOTO 7200
7190     LET U[J-M+1,M]=U[J-M+1,M]+L
7200     LET L=X*L
7210     LET Y=Y*X
7220   NEXT J
7230 NEXT I
7240 FOR I=2 TO M
7250   FOR J=1 TO M-1
7260     LET U[I,J]=U[I-1,J+1]
7270   NEXT J
7280 NEXT I
7290 MAT G=INV(U)
7300 MAT A=G*H
7310 MAT Z=TRN(Y)
7320 MAT W=Z*Y
7330 LET E2=W[1,1]
7340 LET E3=H[1,1]*H[1,1]/(C[5,N+2]+1)
7350 MAT Z=U*A
7360 MAT K=TRN(A)
7370 MAT W=K*Z
7380 LET E4=W[1,1]
7390 LET E7=(E4-E3)/(E2-E3)
7395 IF M-1=0 THEN GOTO 7560
7400 ON M-1 THEN GOTO 7560, 7470
7420 WRITE FILE[2,20+N+F3],Y9,H1,H2,H3,H4,E7,A[1,1],A[2,1],A[3,1],
      A[4,1]
7430 PRINT "CUBIC SOLUTION FOR ";A$
7440 PRINT USING "C=++.##^^^^ ++.##^^^^*A/D++.##^^^^*A/D^2++.##^^^^*
      A/D^3", A[1,1],A[2,1],A[3,1],A[4,1]
7450 PRINT "COEFF. OF DETN. =";E7
7460 GOTO 7610
7470 IF E8=0 THEN GOTO 7500
7480 GOTO 5240
7485 REM RETURN TO SLOPE PROGRAM
7500 WRITE FILE[2,20+N+F3],Y9,H1,H2,H3,H4,E7,A[1,1],A[2,1],A[3,1]
7510 PRINT "QUADRATIC SOLUTION FOR ";A$
7520 PRINT USING "C=++.##^^^^ ++.##^^^^*A/D++.##^^^^*A/D^2",A[1,
        1],A[2,1],A[3,1]
7530 PRINT "COEFF. OF DETN. =";E7
7540 GOTO 7610
7560 WRITE FILE[2,20+N+F3],Y9,H1,H2,H3,H4,E7,A[1,1],A[2,1]
7570 PRINT "LINEAR SOLUTION FOR ";A$
```

```
7580 PRINT USING "C=++.##^^^^ ++.##^^^^*A/D",A[1,1],A[2,1]
7590 PRINT "COEFF. OF DETN. =";E7
7600 GOTO 7610
7601 REM ****ROUTINE TO ORDER STNDS FOR INTERP.
7610 FOR J=1 TO C[5,N+2]-1
7620   FOR X=1 TO C[5,N+2]-J
7630     IF C[(N-1)*10+X]<=C[(N-1)*10+X+1] THEN GOTO 7680
7640     LET K=C[(N-1)*10+X]
7650     LET E3=S[(N-1)*10+X]
7660     LET C[(N-1)*10+X]=C[(N-1)*10+X+1]
7670     LET S[(N-1)*10+X]=S[(N-1)*10+X+1]
7674     LET C[(N-1)*10+X+1]=K
7678     LET S[(N-1)*10+X+1]=E3
7680   NEXT X
7682 NEXT J
7685 IF M<5 THEN GOTO 7700
7690 PRINT "STANDARDS ORDERED FOR INTERPOLATION FOR ";A$
7700 RETURN
7995 REM**********SUBROUTINE TO SMOOTH DATA**************
8000 LET A=B[N,2]
8010 LET D1=B[N,3]
8020 GOSUB 5520
8180 LET E2=0
8190 FOR K=(N-1)*35+1 TO (N-1)*35+35
8195   PRINT FILE[3+N],D[K]
8200   IF D[K]<16383 THEN GOTO 8220
8210   LET E2=E2+1
8220 NEXT K
8230 IF E2=0 THEN GOTO 8400
8240 IF E2>3 THEN GOTO 8820
8250 FOR K=(N-1)*35+1 TO (N-1)*35+35
8360   IF D[K]>=16383 THEN GOTO 8390
8365   REM LOOKING FOR 2 OR MORE OFF-SCALE PTS.
8370 NEXT K
8380 GOTO 8400
8390 IF D[K+1]>=16383 THEN GOTO 8820
8400 LET X1=0
8410 LET F1=0
8420 LET M=0
8430 LET J=0
8450 FOR K=F2-A-1 TO F2-2
8460   IF D[K]=0 THEN GOTO 8490
8470   LET F1=D[K]+F1
8480   LET J=J+1
8490 NEXT K
8492 IF F1>0 THEN GOTO 8500
8494 LET R=0
8495 LET E3=0
8496 LET Q=2
8498 GOTO 8870
8500 LET F1=F1/J
8501 IF T=1 THEN GOTO 8504
8502 IF T<>2 THEN GOTO 8510
8504 LET F=0
8506 GOTO 8520
```

```
8510 LET F=C[1,N+2]+C[2,N+2]*F1+C[3,N+2]*F1^2
8520 IF A=21 THEN LET Y=F2-12
8530 IF A=11 THEN LET Y=F2-7
8535 LET M1=0
8540 FOR K=F2-A-1 TO F2-2
8543   IF D[K]<1 THEN LET D[K]=F1
8545   LET M1=M1+1
8560   LET R[M1]=(K-Y)*F+F1
8570   LET L[M1]=D[K]-R[M1]
8580   LET M=M+L[M1]^2
8590 NEXT K
8600 LET E3=SQR(M/(J-2))
8610 IF E3<=D1 THEN GOTO 8760
8620 LET J=0
8625 LET M1=0
8630 FOR K=F2-1-A TO F2-2
8635   LET M1=M1+1
8640   IF D[K]<1 THEN GOTO 8680
8650   IF ABS(L[M1])<=1.5*E3 THEN GOTO 8680
8660   LET D[K]=0
8670   LET J=J+1
8675   IF J>INT(A/3+.5) THEN GOTO 8735
8680 NEXT K
8690 IF J=0 THEN GOTO 8730
8700 LET X1=X1+J
8710 IF X1>INT(A/3+.5) THEN GOTO 8730
8720 GOTO 8410
8725 REM GO BACK TO SMOOTH AGAIN
8730 IF X1<>0 THEN GOTO 8735
8731 IF E3>5*D1 THEN GOTO 8735
8732 GOTO 8760
8733 REM SCATTER NOISE, NO BIG SPIKES
8735 LET Q=2
8745 GOSUB 9400
8750 GOTO 8780
8760 LET Q=0
8780 LET R=R[M1]
8781 REM
8786 REM
8790 IF T=2 THEN GOTO 8880
8810 GOTO 8870
8815 REM DONE, RETURN
8820 LET Q=1
8825 REM OFF-SCALE PEAKS
8840 IF E2>5 THEN LET E2=5
8850 LET R=16381*E2
8860 IF T=2 THEN GOTO 8880
8870 LET X=R-B
8880 WRITE FILE[0,E1],T,Q,P1,P,T1,T0,C4,S,S1,B,R,X,C,E3,J1
8890 RETURN
9395 REM *************SUBROUTINE TO FIND HIGHEST PEAK************
9400 LET A3=0
9401 LET A5=-1
9405 FOR K=(N-1)*35+2 TO (N-1)*35+34
9410   IF A5>D[K] THEN GOTO 9420
```

```
9415   LET M2=K
9417   LET A5=D[K]
9420 NEXT K
9425 IF D[M2]-D[M2-1]<=5*D1 THEN GOTO 9440
9427 IF D[M2]-D[M2+1]<=5*D1 THEN GOTO 9440
9432 LET A3=A3+1
9433 IF A3>5 THEN GOTO 9440
9434 LET D[M2]=0
9435 GOTO 9401
9440 LET R[M1]=D[M2]
9445 RETURN
9495 REM************SUBROUTINE TO PRINT HEADINGS*****************
9500 PRINT  TAB(28);
9510 FOR I=1 TO NO
9530   PRINT B$[10*(I-1)+1,10*I],
9550 NEXT I
9555 PRINT
9560 RETURN
9595 REM **********SUBROUTINE TO OPEN & READ ANALYT FILE*****
9596 REM ANALYT NO. IS K,RECORD NO. IS E1
9600 LET A$=B$[10*(K-1)+1,10*K]
9610 LET J$="TAAID."
9620 LET J$=J$,A$
9630 OPEN FILE[0,0],J$
9640 READ FILE[0,E1],T,Q,P1,P,T1,T0,C4,S,S1,B,R,X,C,E3,J1
9650 RETURN
9660 END
```

```
0210 IS REFERENCED ON LINES:
    0450

0215 IS REFERENCED ON LINES:
    0240

0300 IS REFERENCED ON LINES:
    0220  0474  1040  1060

0435 IS REFERENCED ON LINES:
    2640  3650  3790  4960  5050
    6030

0440 IS REFERENCED ON LINES:
    2750  2810

0470 IS REFERENCED ON LINES:
    0445

0700 IS REFERENCED ON LINES:
    0105  0740

0710 IS REFERENCED ON LINES:
    0478

0800 IS REFERENCED ON LINES:
    0700  0730

0830 IS REFERENCED ON LINES:
    0760

1000 IS REFERENCED ON LINES:
    0225

1010 IS REFERENCED ON LINES:
    1120

1050 IS REFERENCED ON LINES:
    1020

2600 IS REFERENCED ON LINES:
    0325

3000 IS REFERENCED ON LINES:
    0330

3370 IS REFERENCED ON LINES:
    3010

3410 IS REFERENCED ON LINES:
    3404

3450 IS REFERENCED ON LINES:
    3400

3630 IS REFERENCED ON LINES:
    3647

3640 IS REFERENCED ON LINES:
    3632

3643 IS REFERENCED ON LINES:
    3550

3650 IS REFERENCED ON LINES:
    3460  3642

3710 IS REFERENCED ON LINES:
    3701  3704

3729 IS REFERENCED ON LINES:
    3726

3730 IS REFERENCED ON LINES:
    3728

3759 IS REFERENCED ON LINES:
    3756

3770 IS REFERENCED ON LINES:
    3755  3757  3760

4000 IS REFERENCED ON LINES:
    0350

4310 IS REFERENCED ON LINES:
    4290

4380 IS REFERENCED ON LINES:
    4350

4390 IS REFERENCED ON LINES:
    4320

4430 IS REFERENCED ON LINES:
    4780

4470 IS REFERENCED ON LINES:
    4462

4570 IS REFERENCED ON LINES:
    4540

4580 IS REFERENCED ON LINES:
    4571

4750 IS REFERENCED ON LINES:
    4720
```

```
4800 IS REFERENCED ON LINES:
    4330  4760  4770

4805 IS REFERENCED ON LINES:
    4380  4574  4800  4801

4850 IS REFERENCED ON LINES:
    4680  4802

4880 IS REFERENCED ON LINES:
    4840

4950 IS REFERENCED ON LINES:
    5164  5300

5030 IS REFERENCED ON LINES:
    5070

5060 IS REFERENCED ON LINES:
    5010

5080 IS REFERENCED ON LINES:
    4940

5152 IS REFERENCED ON LINES:
    5100

5180 IS REFERENCED ON LINES:
    5161

5240 IS REFERENCED ON LINES:
    7480

5520 IS REFERENCED ON LINES:
    4040  8020

5535 IS REFERENCED ON LINES:
    5525  5530  5531  5532

5539 IS REFERENCED ON LINES:
    5533

5545 IS REFERENCED ON LINES:
    5780

5550 IS REFERENCED ON LINES:
    5700  5710

5565 IS REFERENCED ON LINES:
    5602  5605

5575 IS REFERENCED ON LINES:
    5539  5568  5760

5590 IS REFERENCED ON LINES:
    5545

5603 IS REFERENCED ON LINES:
    5600

5610 IS REFERENCED ON LINES:
    5555  5585  5590

5620 IS REFERENCED ON LINES:
    5612

5700 IS REFERENCED ON LINES:
    5522  5540

5770 IS REFERENCED ON LINES:
    5730  5740  5750

6000 IS REFERENCED ON LINES:
    0370  0403  6120

6100 IS REFERENCED ON LINES:
    0390

7000 IS REFERENCED ON LINES:
    0500

7025 IS REFERENCED ON LINES:
    5230

7190 IS REFERENCED ON LINES:
    7150

7200 IS REFERENCED ON LINES:
    7180

7470 IS REFERENCED ON LINES:
    7400

7500 IS REFERENCED ON LINES:
    7470

7560 IS REFERENCED ON LINES:
    7395  7400

7610 IS REFERENCED ON LINES:
    7005  7460  7540  7600

7680 IS REFERENCED ON LINES:
    7630

7700 IS REFERENCED ON LINES:
    7685

8000 IS REFERENCED ON LINES:
    2610  3000  6000

8220 IS REFERENCED ON LINES:
    8200
```

```
8390 IS REFERENCED ON LINES:
    8360

8400 IS REFERENCED ON LINES:
    8230  8380

8410 IS REFERENCED ON LINES:
    8720

8490 IS REFERENCED ON LINES:
    8460

8500 IS REFERENCED ON LINES:
    8492

8504 IS REFERENCED ON LINES:
    8501

8510 IS REFERENCED ON LINES:
    8502

8520 IS REFERENCED ON LINES:
    8506

8680 IS REFERENCED ON LINES:
    8640  8650

8730 IS REFERENCED ON LINES:
    8690  8710

8735 IS REFERENCED ON LINES:
    8675  8730  8731

8760 IS REFERENCED ON LINES:
    8610  8732

8780 IS REFERENCED ON LINES:
    8750

8820 IS REFERENCED ON LINES:
    8240  8390

8870 IS REFERENCED ON LINES:
    8498  8810

8880 IS REFERENCED ON LINES:
    8790  8860

9400 IS REFERENCED ON LINES:
    4835  8745

9401 IS REFERENCED ON LINES:
    9435

9420 IS REFERENCED ON LINES:
    9410

9440 IS REFERENCED ON LINES:
    9425  9427  9433

9500 IS REFERENCED ON LINES:
    0205

9600 IS REFERENCED ON LINES:
    0320  2700  3530

A     OCCURS ON LINES:
    4000  4390  4400  4410  4420
    4440  4530  4600  4700  4770
    5560  7300  7350  7360  8000
    8450  8520  8530  8540  8630
    8675  8710

A$    OCCURS ON LINES:
    0080  0180  0190  0410  0485
    3360  3670  3678  4805  5162
    7430  7510  7570  7690  9600
    9620

A2    OCCURS ON LINES:
    0144  0315  2615  3385  3415
    3420  3690  3695  3750  3759
    4015  4920  4990  6015

A3    OCCURS ON LINES:
    3725  3762  3763  5080  5110
    5130  5140  5150  5154  5161
    5180  5190  5192  5194  9400
    9432  9433

A5    OCCURS ON LINES:
    9401  9410  9417

A(    OCCURS ON LINES:
    0050  5240  5250  5260  5267
    7420  7440  7500  7520  7560
    7580

B     OCCURS ON LINES:
    2600  2620  3370  3390  3404
    3408  3409  3420  3630  3700
    3704  3706  3708  3709  3710
    3750  4890  4930  5525  5710
    6020  8870  8880  9640

B$    OCCURS ON LINES:
    0155  0190  0485  3670  9530
    9600
```

```
B[    OCCURS ON LINES:
      0155  0176  0180  0183  0185
      0312  0315  0450  0560  0602
      2600  2615  2640  2680  2720
      2750  2780  3385  3400  3460
      3560  3643  3650  3695  3710
      3717  4000  4010  4015  4920
      4960  4990  5020  5539  5565
      5568  5572  5601  5603  5612
      5613  6015  8000  8010

C     OCCURS ON LINES:
      2620  3630  3706  3750  3759
      4930  8880  9640

C4    OCCURS ON LINES:
      2620  3390  3402  3406  3408
      3415  3420  3630  3690  3700
      3702  3706  3708  3750  3759
      4910  4930  6020  6110  8880
      9640

C[    OCCURS ON LINES:
      0155  0590  0600  4470  4590
      4910  5100  5130  5150  5180
      5190  5192  5240  5250  5260
      5265  7025  7040  7050  7100
      7130  7340  7610  7620  7630
      7640  7660  7674  8510

D1    OCCURS ON LINES:
      4010  4680  4801  8010  8610
      8731  9425  9427

D[    OCCURS ON LINES:
      0155  0235  4287  4290  4350
      4380  4445  4450  4540  4550
      4605  4630  4730  5525  5530
      5531  5532  5700  5710  5730
      5740  5750  8195  8200  8360
      8390  8460  8470  8543  8570
      8640  8660  9410  9417  9425
      9427  9434  9440

E1    OCCURS ON LINES:
      0315  0410  2615  2620  2660
      2680  3385  3390  3402  3406
      3408  3490  3500  3630  3695
      3700  3702  3706  3708  3717
      4015  4920  4930  5568  5572
      6015  6020  8880  9640

E2    OCCURS ON LINES:
      4280  4300  4320  4330  7330
      7390  8180  8210  8230  8240
      8840  8850

E3    OCCURS ON LINES:
      2620  3390  3408  3630  3706
      3708  3750  3759  4573  4660
      4680  4720  4801  4930  6020
      7340  7390  7650  7678  8495
      8600  8610  8650  8731  8880
      9640

E4    OCCURS ON LINES:
      4390  4400  4470  7380  7390

E5    OCCURS ON LINES:
      5200  7015  7050  7130

E7    OCCURS ON LINES:
      5265  7390  7420  7450  7500
      7530  7560  7590

E8    OCCURS ON LINES:
      5210  7020  7470

E[    OCCURS ON LINES:
      0100  0173  0210  0220  0225
      0235  0312  0471  0474  1030
      1055

F     OCCURS ON LINES:
      4430  4450  4462  4464  4470
      4590  4620  8504  8510  8560

F1    OCCURS ON LINES:
      4490  4550  4571  4580  4605
      4620  8410  8470  8492  8500
      8510  8543  8560

F2    OCCURS ON LINES:
      4410  4420  4440  4530  4600
      4700  5610  8450  8520  8530
      8540  8630

F3    OCCURS ON LINES:
      0144  0150  0180  6100  7420
      7500  7560

F[    OCCURS ON LINES:
      0156  2780  5613

G     OCCURS ON LINES:
      7080  7290  7300

G1    OCCURS ON LINES:
      0077  1020  1100

G[    OCCURS ON LINES:
      0060
```

H OCCURS ON LINES:
7090 7300

H1 OCCURS ON LINES:
0490 7420 7500 7560

H2 OCCURS ON LINES:
0490 7420 7500 7560

H3 OCCURS ON LINES:
0490 7420 7500 7560

H4 OCCURS ON LINES:
0490 7420 7500 7560

H[OCCURS ON LINES:
0060 7170 7340

I OCCURS ON LINES:
0170 0173 0174 0176 0180
0183 0185 0190 0200 0440
0445 0450 0470 2630 2640
2650 3410 3415 3420 3440
3450 3460 3480 3510 3520
3560 3632 3640 3643 3730
3750 3759 3770 4950 4960
4980 5000 5010 5020 5030
7040 7050 7060 7100 7120
7130 7230 7240 7260 7280
9510 9530 9550

J OCCURS ON LINES:
0180 0185 0590 0600 0605
3720 3740 3759 3763 4510
4560 4580 4660 4690 4740
4760 4765 5520 5525 5530
5531 5532 5535 5540 5545
5550 5575 5580 5590 5600
5601 5603 5610 5613 5720
5730 5740 5750 5770 7140
7150 7160 7170 7190 7220
7250 7260 7270 7610 7620
7682 8430 8480 8500 8600
8620 8670 8675 8690 8700

J$ OCCURS ON LINES:
0080 0160 0190 0720 0730
3674 3678 3680 9610 9620
9630

J1 OCCURS ON LINES:
2620 3630 3706 3708 3750
3759 4930 6020 8880 9640

K OCCURS ON LINES:
0300 2690 2720 2730 2770
2780 2790 3520 4285 4287
4290 4310 4340 4350 4370
4380 4440 4445 4450 4460
4530 4540 4550 4570 4600
4605 4620 4630 4650 4700
4730 4750 5085 5100 5130
5140 5150 5152 7360 7370
7640 7674 8190 8195 8200
8220 8250 8360 8370 8390
8450 8460 8470 8490 8540
8543 8560 8570 8590 8630
8640 8660 8680 9405 9410
9415 9417 9420 9600

K[OCCURS ON LINES:
0060

L OCCURS ON LINES:
3710 3759 3763 7110 7160
7190 7200

L[OCCURS ON LINES:
0060 4630 4640 4720 6100
6110 8570 8580 8650

M OCCURS ON LINES:
3690 3710 3759 3763 4500
4640 4660 5220 7000 7005
7070 7080 7090 7140 7150
7190 7240 7250 7395 7400
7685 8420 8580 8600

M1 OCCURS ON LINES:
4572 4595 4610 4620 4630
4640 4695 4710 4720 4730
4880 8535 8545 8560 8570
8580 8625 8635 8650 8780
9440

M2 OCCURS ON LINES:
9415 9425 9427 9434 9440

M[OCCURS ON LINES:
0100 5565 5570 5601 5603

N OCCURS ON LINES:
0103 0210 0215 0220 0225
0230 0300 0312 0315 0471
0472 0474 0476 0478 0480
0485 0490 0520 0550 0560
0590 0600 0602 0610 1000
1010 1020 1030 1050 1055
2600 2615 2640 2680 2750

```
      2780   3385   3400   3460   3650
      3670   3695   3710   3717   3763
      4000   4010   4015   4285   4287
      4340   4470   4590   4900   4910
      4920   4960   4990   5100   5130
      5140   5150   5154   5180   5190
      5192   5194   5240   5250   5260
      5265   5267   5525   5530   5531
      5532   5539   5565   5568   5572
      5601   5603   5610   5612   5613
      5700   5710   5730   5740   5750
      6015   6100   7025   7040   7050
      7100   7120   7130   7340   7420
      7500   7560   7610   7620   7630
      7640   7650   7660   7670   7674
      7678   8000   8010   8190   8195
      8250   8510   9405

N0     OCCURS ON LINES:
      0150   0155   0156   0157   0170
      0215   0440   0472   0480   0550
      2630   2690   2770   3450   3510
      3632   4950   5000   9510

N1     OCCURS ON LINES:
      0150   0450   3410   3650   3726
      3729   4940   5085

N2     OCCURS ON LINES:
      0150   0450   3650   3701

N8     OCCURS ON LINES:
      0150   3726   3729

N9     OCCURS ON LINES:
      0150   3726   3727

P      OCCURS ON LINES:
      2620   2660   2680   3390   3402
      3406   3408   3415   3420   3490
      3500   3630   3690   3700   3702
      3706   3708   3750   3759   4930
      4990   6020   8880   9640

P1     OCCURS ON LINES:
      2620   2660   2680   3390   3402
      3406   3408   3415   3420   3490
      3500   3630   3690   3700   3702
      3706   3708   3750   3759   4930
      4990   6020   8880   9640

P[     OCCURS ON LINES:
      0156   0174   0445   0478   1000
      1010   1020   1050

Q      OCCURS ON LINES:
      2620   2660   3010   3390   3402
      3406   3408   3415   3420   3490
      3550   3630   3690   3700   3702
      3706   3708   3750   3759   4820
      4850   4930   6020   8496   8735
      8760   8820   8880   9640

R      OCCURS ON LINES:
      2620   3370   3560   3630   3643
      3750   3759   3763   4880   4890
      4930   6020   8494   8780   8850
      8870   8880   9640

R[     OCCURS ON LINES:
      0070   4572   4620   4630   4730
      4880   8560   8570   8780   9440

S      OCCURS ON LINES:
      2620   3390   3402   3406   3408
      3415   3420   3630   3690   3700
      3702   3706   3708   3750   3759
      4930   6020   8880   9640

S1     OCCURS ON LINES:
      2620   3390   3402   3406   3408
      3415   3420   3630   3690   3700
      3702   3706   3708   3750   3759
      4930   6020   8880   9640

S[     OCCURS ON LINES:
      0157   0600   3763   4900   5010
      5020   5140   5194   7120   7650
      7670   7678

T      OCCURS ON LINES:
      0325   0330   0350   0370   0390
      0403   0410   2620   2660   3390
      3402   3406   3408   3415   3420
      3490   3630   3690   3700   3702
      3706   3708   3750   3755   3756
      3759   3760   3780   4930   5522
      6020   8501   8502   8790   8860
      8880   9640

T0     OCCURS ON LINES:
      2620   3390   3402   3406   3408
      3415   3420   3630   3690   3700
      3702   3706   3708   3750   3759
      4930   6020   8880   9640
```

```
T1    OCCURS ON LINES:
      2620   3390   3402   3406   3408
      3415   3420   3490   3500   3630
      3690   3700   3702   3706   3708
      3750   3759   4470   4590   4805
      4900   4910   4930   4940   4990
      5010   5020   6020   6110   8880
      9640

U     OCCURS ON LINES:
      7070   7290   7350

U[    OCCURS ON LINES:
      0100   7160   7190   7260

W     OCCURS ON LINES:
      7320   7370

W[    OCCURS ON LINES:
      0070   7330   7380

X     OCCURS ON LINES:
      0150   0180   2620   2720   3402
      3404   3408   3409   3630   3702
      3704   3708   3709   3750   3757
      4425   4765   4770   4800   4890
      4900   4930   6020   7025   7030
      7120   7200   7210   7620   7630
      7640   7650   7660   7670   7674
      7678   7680   8870   8880   9640

X1    OCCURS ON LINES:
      8400   8700   8710   8730

Y     OCCURS ON LINES:
      3727   3729   3730   4410   4420
      4450   4620   7030   7130   7170
      7210   7310   7320   8520   8530
      8560

Y9    OCCURS ON LINES:
      0490   7000   7420   7500   7560

Y[    OCCURS ON LINES:
      0070   7050

Z     OCCURS ON LINES:
      7310   7320   7350   7370

Z$    OCCURS ON LINES:
      0080   0180

Z[    OCCURS ON LINES:
      0070
```

*LLL: 1980/4